Electronic Supporting Information For

Nitroiminotriazole (NIT)-based potential solid propellants: Synthesis, characterization and applications

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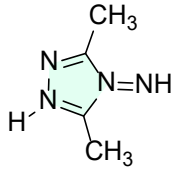
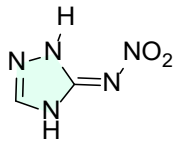
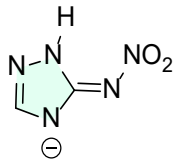
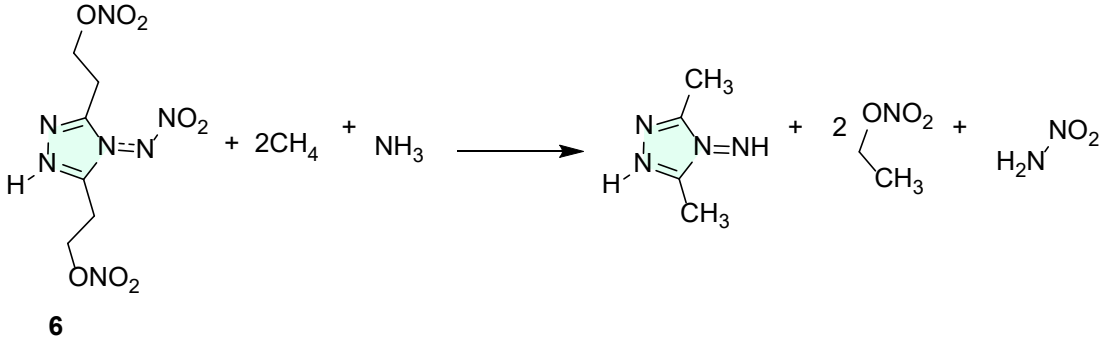
Table S1. Calculated Total Energy (E_0), Zero-point Energy (ZPE), values of Thermal Correction (H_T) and Enthalpy of Formation ($\Delta H_f°$ (g)) of the title compounds using B3LYP/6-31+G**//MP2/6-311++G** level of theory (Isodesmic).

Compounds	E_0 [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	$\Delta H_f°$ (g) kJ/mol	$\Delta H_{sub}°$ kJ/mol	$\Delta H_f°$ (s) kJ/mol
CH_4	-40.39849	0.044791	0.003812	-74.60	----	----
NH_3	-56.43462	0.034377	0.003818	-45.90	----	----
NH_2NO_2	-260.5541444	0.038264	0.004344	-6.10	----	----
$CH_3CH_2ONO_2$	-358.7000232	0.081984	0.006662	-147.77	----	----
	-374.9641434	0.130901	0.009000	991.82	----	----
	-500.9635448	0.079025	0.007837	240.11	89.86	150.25
	-500.439275	0.065614	0.007938	70.13	----	----
6	-1215.984062	0.205417	0.02066	810.68	75.39	735.29
8 ($^+NH_3NH_2$)	----	----	----	840.13	542.44	297.69
9 ($^+NH_3OH$)	----	----	----	739.62	541.55	198.07
10 (NH_4^+)	----	----	----	696.53	554.15	142.38
11 (K^+)	----	----	----	571.23	563.39	7.84
12 (Na^+)	----	----	----	655.13	574.30	80.83

[a] Data are from Ref. [D. R. Lide ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version **2008**), CRC Press/Taylor and Francis, Boca Raton, FL.] [b]Obtained at G2 level. [c]Calculated using isodesmic equation as shown in Figure S1.

The gas-phase enthalpies of formation $\Delta_fH°(g)$ were predicted using Gaussian 03 program[1] based on isodesmic equations (Figure S1).



6

Fig. S1: Isodesmic reactions for the compounds **6**.

Subsequently, for compound **5**, the solid-phase enthalpy of formation $\Delta H_f°$ (s) was calculated by using equation 1.[2-3]

$\Delta H_f^\circ(s) = \Delta H_f^\circ(g) - \Delta H_{sub}$ (1)

Where, $\Delta H_f^\circ(s)$ is the solid phase enthalpy of formation, $\Delta H_f^\circ(g)$ is gas phase enthalpy of formation and ΔH_{sub} is the enthalpy of sublimation.

The enthalpy of sublimation was estimated using equation 2 based on Trouton's rule:[3,4]

$\Delta H_{sub} = 0.188 \times T/kJmol^{-1}K^{-1}$ (2)

where, *T*, is either the melting point (mp) or the decomposition temperature (T_d), when melting does not occur before decomposition.

For salts **8-12**, the solid phase enthalpies of formation were obtained using the Born-Haber energy cycle.[3]

The bond dissociation energies (BDEs) of compound **5** were estimated according to equ. 3.

$BDE\ [AB] = E_0\ [A.] + E_0\ [B.] - E_0\ [AB]$ (3)

where, BDE [AB] is bond dissociation energy and E_0 [A.] and E_0 [B.] are the energies of individual homolytic part and E_0 [AB] is the total energy of the individual molecule.

Table S2. The standard enthalpies of combustion, $\Delta H_f^\circ{}_{(combust)}$, for the title compounds were calculated by equations 4-8.

$\Delta H_f^\circ{}_{(combust)} = \Sigma\Delta H_f^\circ{}_{(products)} - \Sigma\Delta H_f^\circ{}_{(reactants)}$ (4)

RDX = $C_3H_6N_6O_6\ (s) + 1.5\ O_2\ (g) \longrightarrow 3CO_2\ (g) + 3H_2O\ (g) + 3N_2\ (g)$ (5)

TNT = $C_7H_5N_3O_6\ (s) + 5.25O_2\ (g) \longrightarrow 7CO_2\ (g) + 2.5H_2O\ (g) + 1.5N_2\ (g)$ (6)

5 = $C_2H_3N_5O_2\ (s) + 0.75\ O_2\ (g) \longrightarrow 2CO_2\ (g) + 1.5H_2O\ (g) + 2.5N_2\ (g)$ (7)

6 = $C_6H_9N_7O_8\ (s) + 4.25\ O_2\ (g) \longrightarrow 6CO_2\ (g) + 4.5H_2O\ (g) + 3.5N_2\ (g)$ (8)

The standard enthalpy of formation for CO_2 ($\Delta H_f^\circ{}_{(CO2)} = -393.51\ kJmol^{-1}$); H_2O ($\Delta H_f^\circ{}_{(H2O)} = -243.015\ kJmol^{-1}$).

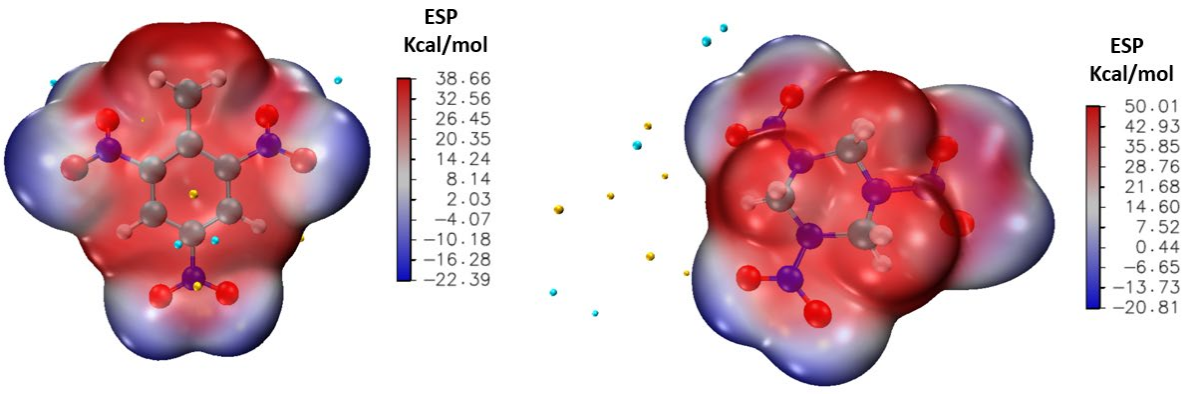


Fig. S2: Computed electrostatic potential (ESP) maps of TNT and RDX.

Table S3. Comparison of the ratio of positive and negative ESPs and the surface area of ESPs of compounds and positive variance, total variance, balance of charges and product of total variance and balance of charges.

Compounds	A_{tot}[a] Å^2	A_{pos}[b] Å^2	A_{neg}[c] Å^2	$ratio_{pos}$ (%)	$ratio_{neg}$ (%)	$\sigma^2_{tot}\upsilon$[d] (kcal/mol)
5	144.74	76.25	68.49	52.68	47.32	69.93
6	298.47	158.36	140.11	53.06	46.94	86.31
11	475.34	262.21	213.13	55.16	44.84	197.45
RDX	209.49	116.77	92.72	55.74	44.26	27.29

[a]SA_{tot} = Total surface area. [b]SA_{pos} = positive surface area. [c]SA_{neg} = Negative surface area. [d]Ratio of positive surface area [e d]Ratio of negative surface area. [g]Product of total variance and balance of charges.

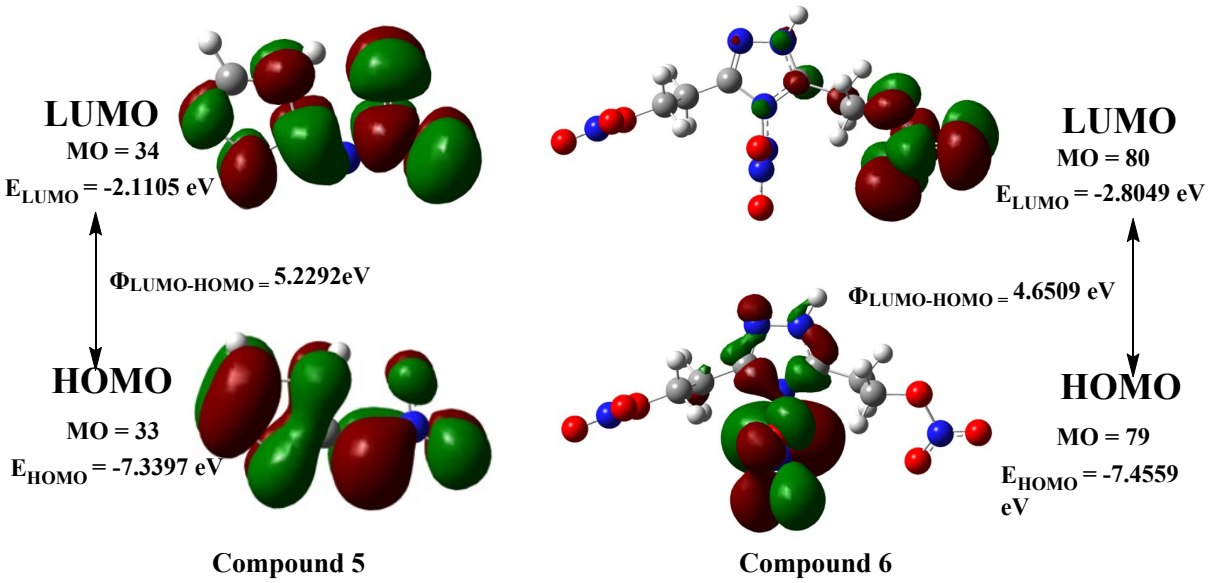


Fig. S3: HOMO and LUMO energies of compounds **5** and **6**.

EXPERIMENTAL SECTION

General Methods

All reagents and solvents were used as received unless otherwise specified (AKSci, Sigma-Aldrich, Acros Organics, VWR). The densities of the new compounds were obtained at 25 °C with a Micromeritics Accupyc II 1340 gas pycnometer. The thermal stability (melting and decomposition points) was measured by heating individual samples from 35 °C to 400 °C at the heating rates of 5 °C and 10 °C min^{-1} using a

differential scanning calorimeter (DSC, TA Instruments Company, Model: Q2000) and thermogravimetric analysis (TGA, TA Instruments Company, Model: Q50). The FTIR spectra were recorded with KBr plates on a Thermo Nicolet AVATAR 370 spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on a 500 MHz (Bruker) nuclear magnetic resonance spectrometer operating at 500.19 and 125.77 MHz, respectively, using DMSO-d_6 as the solvent and locking solvent. The ^{15}N NMR spectra were recorded on a 500.19 MHz (Bruker 500) nuclear magnetic resonance operating at 50.70 MHz. As external standards, the chemical shifts are given relative to tetramethylsilane (^{1}H, ^{13}C) and nitromethane (^{15}N). Elemental analyses (C, H, N) were performed using a Vario Micro cube Elemental Analyser. The friction sensitivities (FS) and impact sensitivities (IS) were measured with a standard BAM friction tester and BAM drop hammer.[5] Crystals of **6, 11** and **14** was mounted on a nylon loop with Paratone oil on an XtaLAB Synergy, Dualflex, HyPix diffractometer at 100 K. The structures were solved with the ShelXT[6-9] solution program using dual methods and Olex2.[10] The model was refined with ShelXL34 using full matrix least squares minimization on F^2.

Caution! The compounds studied in the present work are potentially high-energy materials. Therefore, it is strongly recommended that these compounds should be synthesized and handled with extreme care with all the standard safety precautions employed.

2,4-Dihydro-3H-1,2,4-triazol-3-ylidene-nitramide **(5).** Fuming HNO_3 (25.2 mL, 600 mmol, 10 equiv.) was cooled at 0 °C and H_2SO_4 (98%, 32.0 mL, 600 mmol, 10 equiv.) was added dropwise. The resulting mixture was stirred for 30 min at the same temperature. Compound **7** (5.04 g, 60 mmol, 1 equiv.) was added portion-wise. The resulting reaction mixture was stirred at room temperature for 10 h and poured into ice-cold water. The white solid which was formed was filtered off, dried, and triturated with

acetonitrile. Crystalline, white solid; Yield: 7.040 g, 91%, DSC (5 °C min^{-1}): $T_{d\ (onset)}$ 205 °C; IR (KBr pellet) ṽ 3121 (s), 2951 (s), 1591 (s), 1541 (s), 1462 (s), 1403 (m), 1316 (s), 1281 (s), 1098 (m), 1058 (m), 997 (w), 951 (m), 869 (m), 849 (m), 776 (w), 719 (m) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 8.44 (s, 1H), 14.14 (s, 2H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 139.2, 152.4; Elemental analysis: calcd (%) for $C_2H_3N_5O_2$ (129.08): C, 18.61; H, 2.34; N, 54.26. Found C, 18.70; H, 2.55; N, 54.86.

(4-(Nitroamino)-4H-1λ⁴,2,4-triazole-3,5-diyl)bis(ethane-2,1-diyl) dinitrate (6). H_2SO_4 (98%, 2.7 mL, 50 mmol, 10 equiv.) was cooled at 0 °C and fuming HNO_3 (2.1 mL, 50 mmol, 10 equiv.) was added dropwise. The resulting mixture was stirred for 15 min at the same temperature. Compound **14** (0.860 g, 5 mmol, 1 equiv.) was added portion-wise. The resulting reaction mixture was stirred at room temperature for 6 h and poured into ice-cold water and extracted with DCM. The solvent was evaporated in air and a colorless solid was further purified by the trituration with hexane. Crystalline, colorless solid; Yield: 1.23 g, 80%, DSC (5 °C min^{-1}): T_m 121 °C; $T_{d\ (onset)}$ 134 °C; IR (KBr pellet) ṽ 3026 (m), 2995 (m), 2967 (m), 2901 (s), 2703 (s), 2639 (s), 1622 (s), 1557 (m), 1460 (s), 1406 (s), 1335 (s), 1278 (s), 1254 (s), 1189 (m), 1104 (m), 1048 (m), 1010 (s), 978 (s), 889 (s), 846 (s), 773 (s), 752 (s), 715 (m), 699 (m) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 3.26 (t, J = 6.8Hz, 4H), 4.85 (t, J = 6.8Hz, 4H), 10.4 (brs, 1H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 21.9, 68.3, 151.1; ^{15}N NMR (50.70 MHz, DMSO-d_6): δ -3.47, -42.17, -128.58, -134.10, -168.62; Elemental analysis: calcd (%) for $C_6H_9N_7O_8$ (307.18): C, 23.46; H, 2.95; N, 31.92. Found C, 23.54; H, 2.88; N, 32.67.

General procedure for the syntheses of salts 8-12.

Compound **5** (1.290 g, 10 mmol, 1 equiv.) was dissolved in water (5 mL), and hydrazine hydrate or hydroxylamine monohydrate or aq ammonia or KOH or NaOH (50 mmol, 5 equiv.) was added dropwise; a white precipitate was formed, and the suspension was

stirred for 5 h at room temperature. The solvent was evaporated, and the solid taken up in acetonitrile. The reaction mixture was filtered to give a crude compound, which was further purified by trituration with acetonitrile.

Hydrazinium-5-(nitroimino)-1,5-dihydro-1,2,4-triazol-4-ide **(8).** Crystalline, light-yellow solid; Yield: 1.58 g, 98%, DSC (5 °C min^{-1}): $T_{d\ (onset)}$ 211 °C. IR (KBr pellet) ṽ 3283-2775 (brs),1871 (s), 1829 (m), 1707 (w), 1527 (s), 1483 (s), 1341 (s), 1306 (s), 1283 (s), 1236 (s), 1215 (s), 1110 (s), 1064 (s), 1006 (s), 976 (s), 918 (s), 854 (s) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 7.69 (s, 1H), 8.66 (s, 5H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 148.6, 156.7; Elemental analysis: calcd (%) for $C_2H_7N_7O_2$ (161.13): C, 14.91; H, 4.38; N, 60.85. Found C, 15.40; H, 4.09; N, 58.77.

Hydroxylammonium-5-(nitroimino)-1,5-dihydro-1,2,4-triazol-4-ide **(9).** Crystalline, light-yellow solid; Yield: 1.89 g, 97%, DSC (5 °C min^{-1}) $T_{d\ (onset)}$ 213 °C. IR (KBr pellet) ṽ 3274-2464 (brs), 1610 (m), 1497 (s), 1342 (s), 1259 (s), 1103 (s), 1076 (s), 1021 (m), 1004 (m), 976 (s), 924 (m), 891 (m), 868 (m), 767 (m), 729 (s) cm^{-1}. ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 7.67 (s, 1H), 9.21 (br s, 4H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 148.4, 156.6; Elemental analysis: calcd (%) for $C_2H_9N_7O_4$ (195.14): C, 12.31; H, 4.65; N, 50.25. Found C, 12.91; H, 4.73; N, 50.41.

Ammonium-5-(nitroimino)-1,5-dihydro-1,2,4-triazol-4-ide **(10).** Crystalline, colorless solid; Yield: 1.43 g, 98%, DSC (5 °C min^{-1}): $T_{d\ (onset)}$ 218 °C; IR (KBr pellet) ṽ 3184-2757 (brs), 1528 (s), 1454 (s), 1343 (s), 1283 (s), 1236 (s), 1106 (s), 1062 (s), 1006 (m), 974 (s), 918 (s), 852 (m), 771 (s), 731 (s) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 7.40 (s, 4H), 7.83 (s, 1H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 146.3, 155.7; Elemental analysis: calcd (%) for $C_2H_6N_6O_2$ (146.11): C, 16.44; H, 4.14; N, 57.52. Found C, 16.44; H, 4.21; N, 57.92.

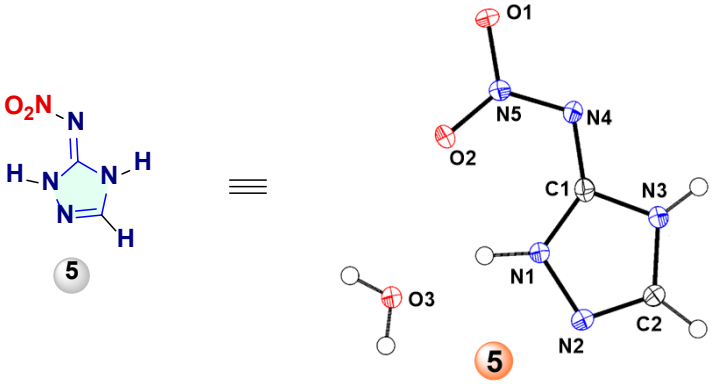
Potassium-5-(nitroimino)-1,5-dihydro-1,2,4-triazol-4-ide (11). Crystalline, light brown solid; Yield: 3.70 g, 99%, DSC (5 °C min^{-1}): $T_{d\ (onset)}$ 258 °C; IR (KBr pellet) ṽ 3132 (w), 158 (s), 1474 (s), 1441 (s), 1382 (s), 1339 (s), 1257 (s), 1204 (w), 1185 (m), 1094 (w), 1062 (s), 995 (s), 893 (m), 857 (m), 802 (w), 747 (m), 718 (m); ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 7.55 (s, 1H), 12.78 (brs, 1H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 148.8, 157.1; Elemental analysis: calcd (%) for $C_4H_4K_3N_{10}O_4$ (373.44): C, 12.87; H, 1.08; N, 37.51. Found C, 12.37; H, 0.90; N, 36.20.

Sodium--5-(nitroimino)-1,5-dihydro-1,2,4-triazol-4-ide (12·H_2O). Crystalline, light brown solid; Yield: 1.87 g, 98%, DSC (5 °C min^{-1}): $T_{d\ (onset)}$ 378 °C; IR (KBr pellet) ṽ 3337 (s), 3096 (s), 1682 (m), 1440 (s), 1390 (s), 1342 (s), 1312 (s), 1263 (s), 1202 (s), 1069 (s), 1041 (s), 1001 (s), 891 (m), 861 (s), 724 (s), 686 (s) cm^{-1}; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 7.44 (s, 1H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 148.8, 157.0; Elemental analysis: calcd (%) for $C_2HNaN_5O_2.H_2O$ (191.06): C, 12.57; H, 1.58; N, 36.36. Found C, 12.80; H, 1.51; N, 36.53.

2,2'-(4-amino-4H-1,2,4-triazole-3,5-diyl)bis(ethan-1-ol) (13). Commercially available 3-hydroxypropanenitrile **13**, (3.550 g, 50 mmol, 1 equiv), sulfur powder (0.960 g, 30 mmol, 0.6 equiv) and hydrazine monohydrate (12.5 g, 250 mmol, 5 equiv) heated at 80 °C in ethanol for 10 h. The resulting reaction mixture was cooled, ethanol was evaporated, and sulfur was removed by washing with toluene. The crude residue was further purified by recrystallization with ethanol. Crystalline, colorless solid; Yield: 3.70 g, 86%, DSC (5 °C min^{-1}): T_m = 150 °C (melting point); IR (KBr pellet) ṽ 3321-2692 (brs), 1614 (s), 1531 (s), 1476 (s), 1423 (s), 1388 (s), 1359 (s), 1323 (m), 1285 (m), 1209 (m), 1055 (s), 974 (s), 875 (s), 802 (m), 787 (m), 743 (s), 702 (m) cm^{-1} ; ^{1}H NMR (500.19 MHz, DMSO-d_6): δ 2.85 (t, *J* = 6.8Hz, 4H), 3.71 (t, *J* = 6.8Hz, 4H), 4.99 (brs, 2H), 5.81 (brs, 2H); ^{13}C NMR (125.77 MHz, DMSO-d_6): δ 21.9, 68.3, 151.1; ^{15}N NMR (50.70

MHz, DMSO-d_6): δ -79.23, -200.75, -319.34; Elemental analysis: calcd (%) for $C_6H_{12}N_4O_2$ (172.19): C, 41.85; H, 7.02; N, 32.54. Found C, 41.78; H, 7.43; N, 33.13.

Table S4. Single crystal X-ray data and structure refinement for compound **5**.[6-10]



Compound	**5**
CCDC	2303917
Formula	$C_4H_{10}N_{10}O_6$
$D_{calc.}$/ g cm^{-3}	1.740
m/mm^{-1}	1.396
Formula Weight	294.22
Colour	colourless
Shape	irregular-shaped
Size/mm^3	0.15×0.12×0.04
T/K	100.00(10)
Crystal System	monoclinic
Flack Parameter	-0.17(18)
Hooft Parameter	-0.27(16)
Space Group	$P2_1$
a/Å	5.16088(12)
b/Å	8.67413(16)
c/Å	6.54739(15)
a/°	90
b/°	106.652(2)
g/°	90
V/Å^3	280.810(11)
Z	1
Z'	0.5
Wavelength/Å	1.54184
Radiation type	Cu K_a
Q_{min}/°	7.059
Q_{max}/°	80.067
Measured Refl's.	2882
Indep't Refl's	1171
Refl's I≥2 s(I)	1153
R_{int}	0.0280
Parameters	107
Restraints	1
Largest Peak	0.191
Deepest Hole	-0.259
GooF	1.064
wR_2 (all data)	0.0754
wR_2	0.0751
R_1 (all data)	0.0285
R_1	0.0283

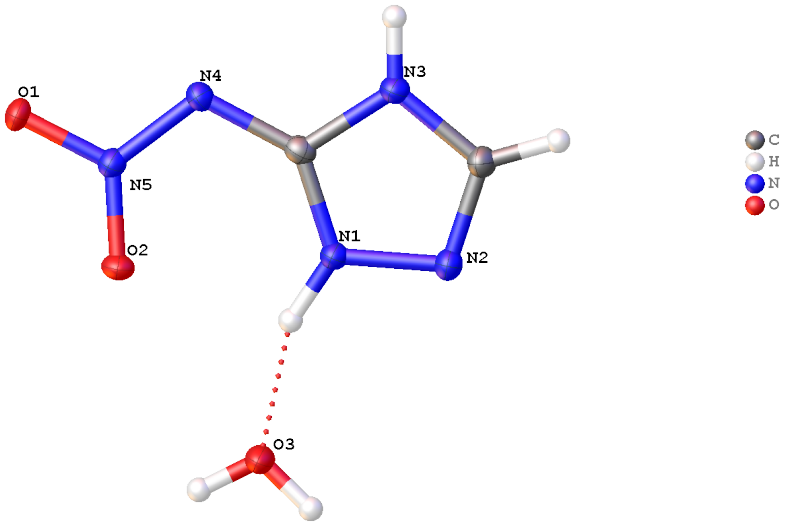


Fig. S4. Drawing at 50% ellipsoids with hetero atoms labelled and hydrogen atoms on the nitrogen atoms found and refined isotropically.

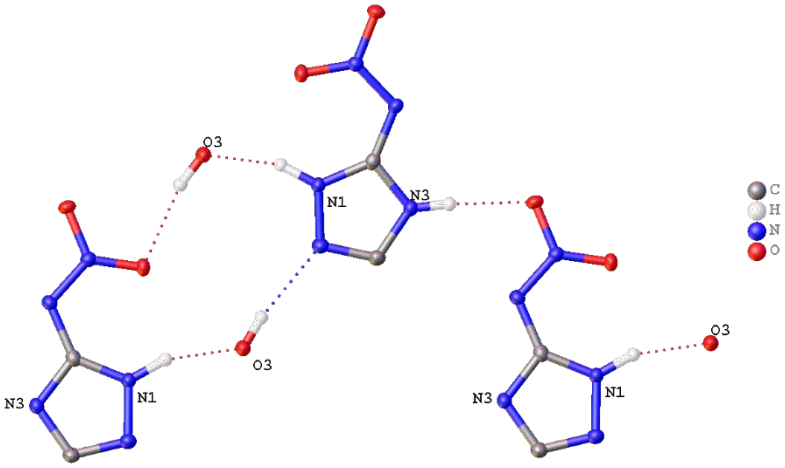


Fig. S5. The following hydrogen bonding interactions with a maximum D-D distance of 2.9 Å and a minimum angle of 120 ° are present in compound **5**: O3–O2_*1: 2.868 Å, N3–O1*_2: 2.794 Å, N1–O3: 2.678 Å.

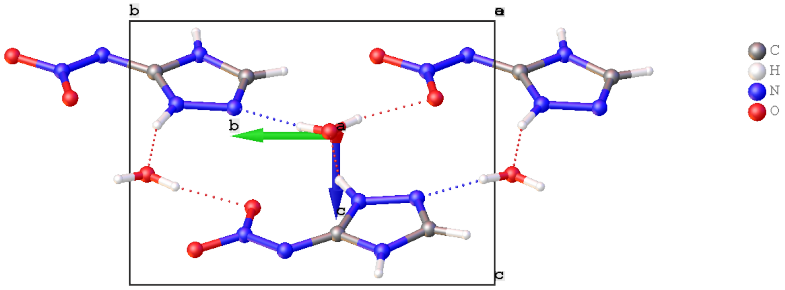


Fig. S6. Packing diagram of compound **5** viewed along the a axis

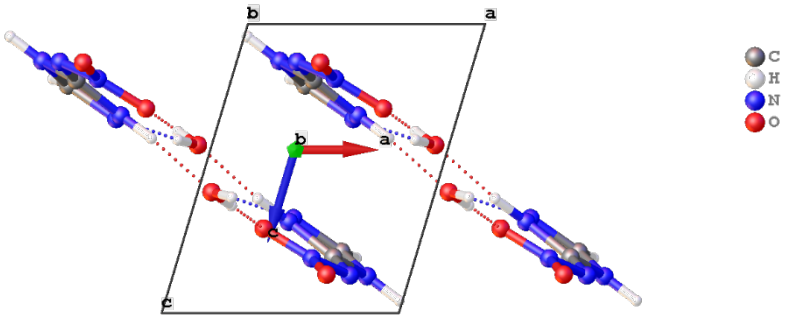


Fig. S7. Packing diagram of compound **5** viewed along the b axis

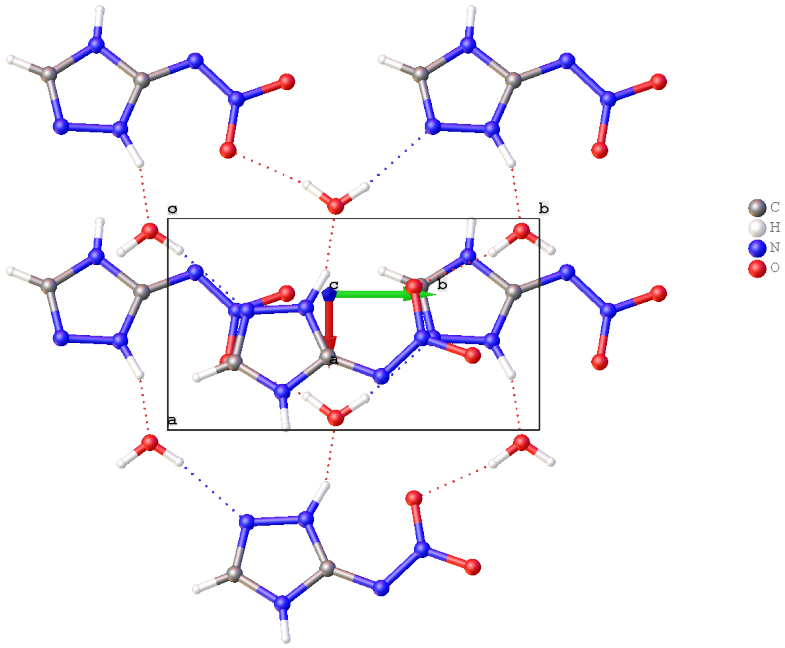


Fig. S8. Packing diagram of compound **5** viewed along the c axis

Table S5: Bond Lengths in Å for compound **5**.

Atom	Atom	Length/Å
O1	N5	1.268(3)
O2	N5	1.246(3)
N5	N4	1.322(3)
N4	C1	1.356(3)
N3	C1	1.357(3)
N3	C2	1.354(4)
N1	N2	1.374(3)
N1	C1	1.337(3)
N2	C2	1.307(3)

Table S6: Bond Angles in ° for compound **5**.

Atom	Atom	Atom	Angle/°
O1	N5	N4	115.74(19)
O2	N5	O1	120.29(19)
O2	N5	N4	124.0(2)
N5	N4	C1	114.8(2)
C2	N3	C1	107.29(19)
C1	N1	N2	111.4(2)
C2	N2	N1	104.2(2)
N4	C1	N3	119.1(2)
N1	C1	N4	135.4(2)
N1	C1	N3	105.5(2)
N2	C2	N3	111.6(2)

Table S7: Torsion Angles in ° for compound **5**.

Atom	Atom	Atom	Atom	Angle/°
O1	N5	N4	C1	-179.73(19)
O2	N5	N4	C1	1.3(3)
N5	N4	C1	N3	-175.5(2)
N5	N4	C1	N1	5.3(4)
N1	N2	C2	N3	0.2(3)
N2	N1	C1	N4	179.9(2)
N2	N1	C1	N3	0.6(3)
C1	N3	C2	N2	0.2(3)
C1	N1	N2	C2	-0.5(3)
C2	N3	C1	N4	-179.9(2)
C2	N3	C1	N1	-0.5(3)

Table S8: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **5**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

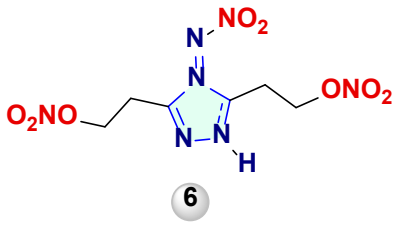
Atom	x	y	z	U_{eq}
H2	7516.94	788.47	8100.6	21
H3A	-1500(80)	5310(50)	4000(60)	23(8)
H3B	-1590(80)	3760(50)	3720(60)	29(9)
H3	9850(80)	3180(60)	9560(70)	44(11)
H1	2620(80)	4240(50)	6050(60)	35(10)

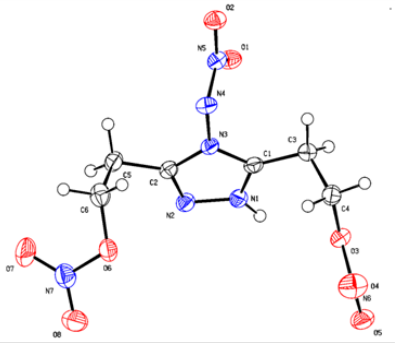
Table S9: Hydrogen Bond information for compound **5**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O3	H3B	O2[1]	0.85(4)	2.04(4)	2.868(3)	167(4)
N3	H3	O1[2]	0.88(4)	1.92(4)	2.794(3)	175(4)
N1	H1	O3	0.95(4)	1.77(4)	2.678(3)	159(4)

[1]-x,-1/2+y,1-z; [2]2-x,-1/2+y,2-z

Table S10. Single crystal X-ray data and structure refinement for compound **6**.[6-10]





Formula	$C_6H_9N_7O_8$
$D_{calc.}$/ g cm^{-3}	1.699
m/mm^{-1}	1.395
Formula Weight	307.20
Color	yellow
Shape	block-shaped
Size/mm^3	0.12×0.05×0.02
T/K	100.00(10)
Crystal System	orthorhombic
Space Group	*Pbca*
a/Å	6.2321(2)
bÅ	10.9604(3)
c/Å	35.1593(9)
α/°	90
β/°	90
γ/°	90
V/Å^3	2401.60(12)
Z	8
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K$_a$
Q_{min}/°	2.513
Q_{max}/°	77.295
Measured Refl's.	8297
Indep't Refl's	2332
Refl's I≥2 s(I)	2042
R_{int}	0.0453
Parameters	194
Restraints	0
Largest Peak	0.406
Deepest Hole	-0.264
GooF	1.055
wR_2 (all data)	0.1168
wR_2	0.1124
R_1 (all data)	0.0502
R_1	0.0432

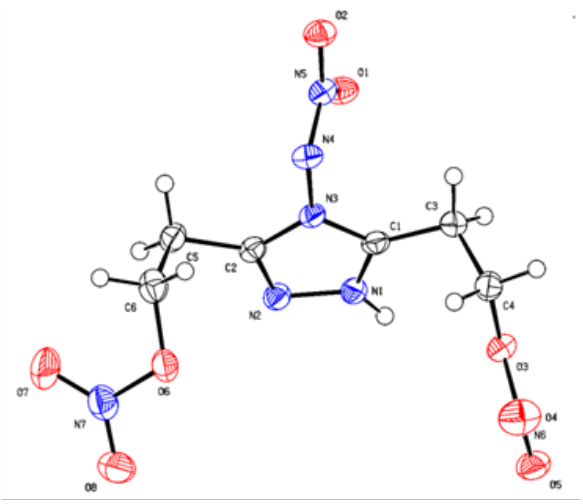


Fig. S9. Molecular structure (thermal ellipsoid plot (50%) of compound **6** (CCDC, 2296314).

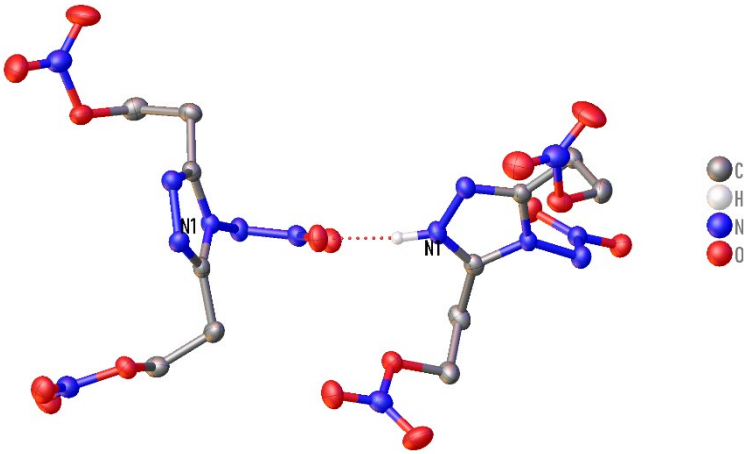


Fig. S10. The following hydrogen bonding interactions with a maximum D-D distance of 3.1 Å and a minimum angle of 110 ° are present in compound **6**: N1–O1_*1: 2.685 Å.*

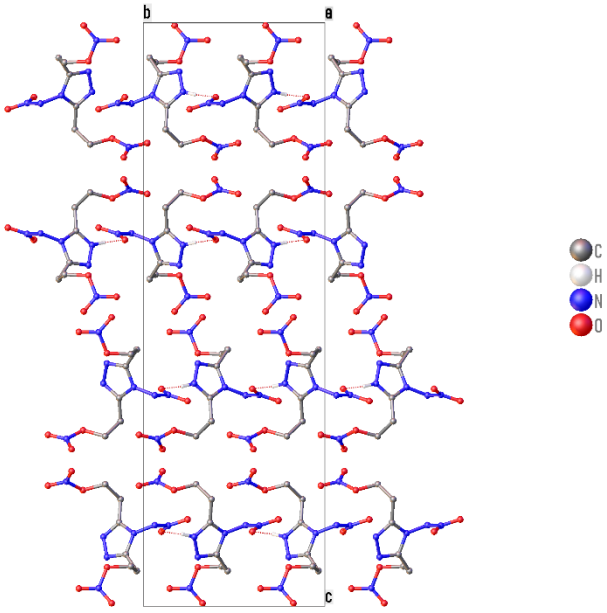


Fig. S11. Packing diagram of compound **6**.

Table S11: Bond Lengths in Å for compound **6.**

Atom	Atom	Length/Å
O1	N5	1.265(2)
O2	N5	1.236(2)
O3	N6	1.382(2)
O3	C4	1.448(2)
O4	N6	1.206(2)
O5	N6	1.200(2)
O6	N7	1.396(2)
O6	C6	1.449(3)
O7	N7	1.197(2)
O8	N7	1.204(2)
N1	N2	1.373(2)
N1	C1	1.308(3)
N2	C2	1.306(2)
N3	N4	1.412(2)
N3	C1	1.344(2)
N3	C2	1.377(2)
N4	N5	1.336(2)
C1	C3	1.479(3)
C2	C5	1.490(3)
C3	C4	1.521(3)
C5	C6	1.527(3)

Table S12: Bond Angles in ° for compound **6.**

Atom	Atom	Atom	Angle/°
N6	O3	C4	113.64(15)
N7	O6	C6	114.91(15)
C1	N1	N2	112.62(16)
C2	N2	N1	103.95(15)
C1	N3	N4	126.22(16)
C1	N3	C2	107.35(15)
C2	N3	N4	126.09(15)
N5	N4	N3	107.71(14)
O1	N5	N4	121.58(15)
O2	N5	O1	121.50(15)
O2	N5	N4	116.90(15)
O4	N6	O3	118.39(16)
O5	N6	O3	113.60(17)
O5	N6	O4	128.01(18)
O7	N7	O6	118.52(18)
O7	N7	O8	129.0(2)
O8	N7	O6	112.50(17)
N1	C1	N3	105.77(17)
N1	C1	C3	127.49(18)
N3	C1	C3	126.73(18)
N2	C2	N3	110.30(16)
N2	C2	C5	126.08(17)
N3	C2	C5	123.44(16)
C1	C3	C4	111.44(16)

Atom	Atom	Atom	Angle/°
O3	C4	C3	104.98(16)
C2	C5	C6	110.28(16)
O6	C6	C5	110.82(16)

Table S13: Torsion Angles in ° for compound **6**.

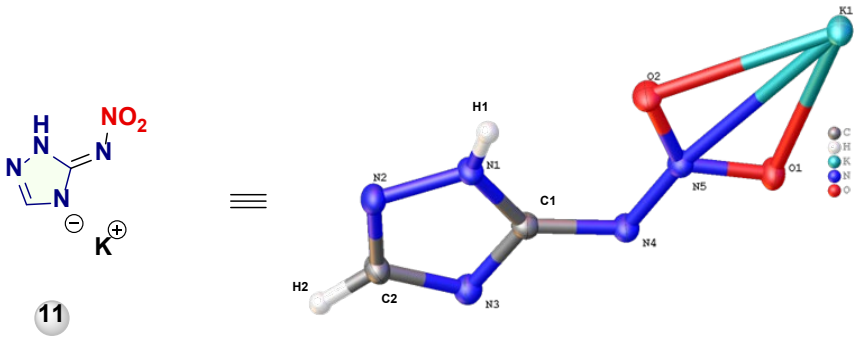
Atom	Atom	Atom	Atom	Angle/°
N1	N2	C2	N3	-0.4(2)
N1	N2	C2	C5	-175.67(18)
N1	C1	C3	C4	-75.7(3)
N2	N1	C1	N3	-0.2(2)
N2	N1	C1	C3	178.39(18)
N2	C2	C5	C6	94.8(2)
N3	N4	N5	O1	-3.0(2)
N3	N4	N5	O2	178.79(15)
N3	C1	C3	C4	102.7(2)
N3	C2	C5	C6	-79.9(2)
N4	N3	C1	N1	-173.61(16)
N4	N3	C1	C3	7.8(3)
N4	N3	C2	N2	173.86(16)
N4	N3	C2	C5	-10.7(3)
N6	O3	C4	C3	-167.77(15)
N7	O6	C6	C5	-89.1(2)
C1	N1	N2	C2	0.4(2)
C1	N3	N4	N5	72.5(2)
C1	N3	C2	N2	0.3(2)
C1	N3	C2	C5	175.71(17)
C1	C3	C4	O3	71.6(2)
C2	N3	N4	N5	-99.9(2)
C2	N3	C1	N1	0.0(2)
C2	N3	C1	C3	-178.65(18)
C2	C5	C6	O6	-59.1(2)
C4	O3	N6	O4	3.1(2)
C4	O3	N6	O5	-177.13(16)
C6	O6	N7	O7	-3.7(3)
C6	O6	N7	O8	176.29(17)

Table S14: Hydrogen Bond information for compound **6**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1	O1[1]	0.90(3)	1.79(3)	2.685(2)	171(3)

[1]1/2-x,-1/2+y,

Table S15. Single crystal X-ray data and structure refinement for compound **11**.[6-10]



Formula	$C_2H_2KN_5O_2$
$D_{calc.}$/ g cm^{-3}	2.009
m/mm^{-1}	8.001
Formula Weight	167.19
Colour	colourless
Shape	irregular-shaped
Size/mm^3	0.16×0.14×0.09
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	-0.016(9)
Hooft Parameter	-0.011(4)
Space Group	$P2_1$
a/Å	4.07223(5)
b/Å	10.00743(14)
c/Å	6.99455(9)
α/°	90
β/°	104.2041(13)
γ/°	90
V/Å^3	276.331(6)
Z	2
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K_a
Q_{min}/°	6.528
Q_{max}/°	79.665
Measured Refl's.	5570
Indep't Refl's	1123
Refl's I≥2 s(I)	1117
R_{int}	0.0280
Parameters	96
Restraints	1
Largest Peak	0.249
Deepest Hole	-0.288
GooF	1.128
wR_2 (all data)	0.0708
wR_2	0.0707
R_1 (all data)	0.0254
R_1	0.0253

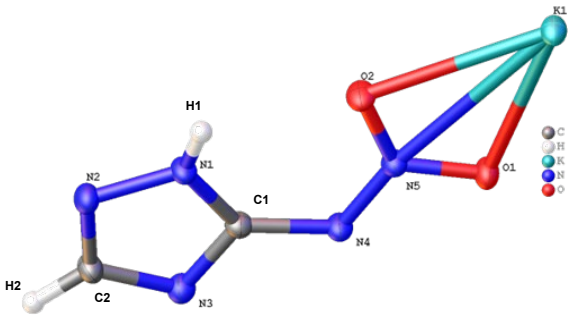


Fig. S12. Molecular structure (thermal ellipsoid plot (50%) of compound **11** (CCDC, 2296315).

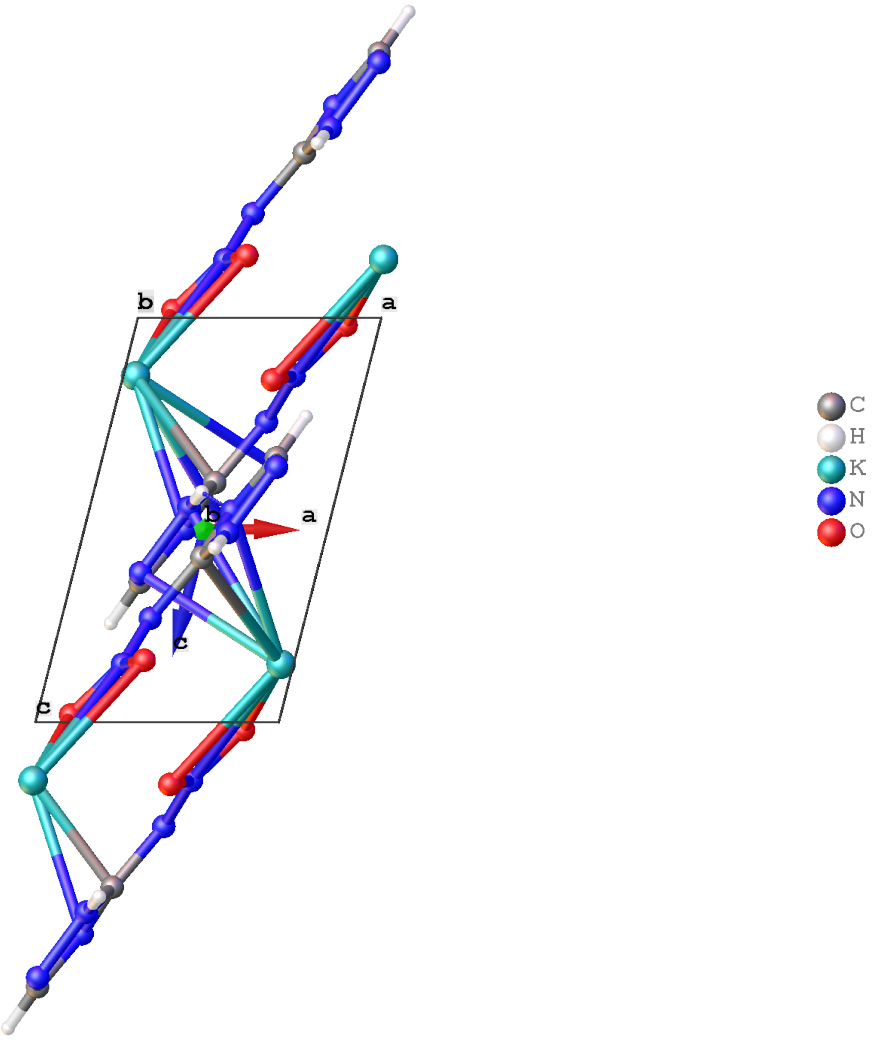


Fig. S13. Packing diagram of compound **11** viewed along the b axis

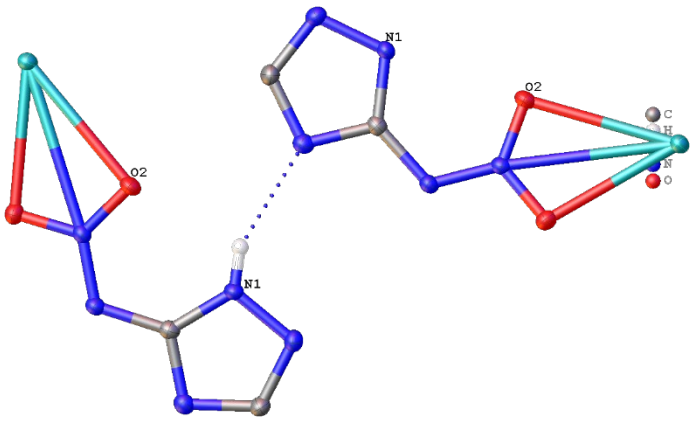


Fig. S14. The following hydrogen bonding interactions with a maximum D-D distance of 3.1 . Å and a minimum angle of 110 ° are present in compound **11**: N1–O2: 2.624 Å, N1–N3_*1: 2.924 Å.*

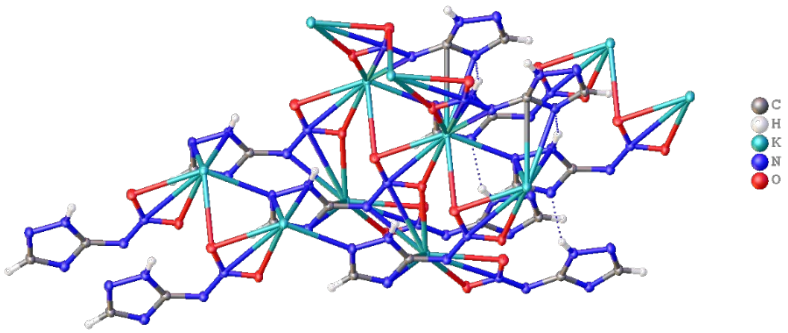


Fig S15. Drawing at 50% ellipsoids (compound **11)** showing the polymeric nature of the compound.

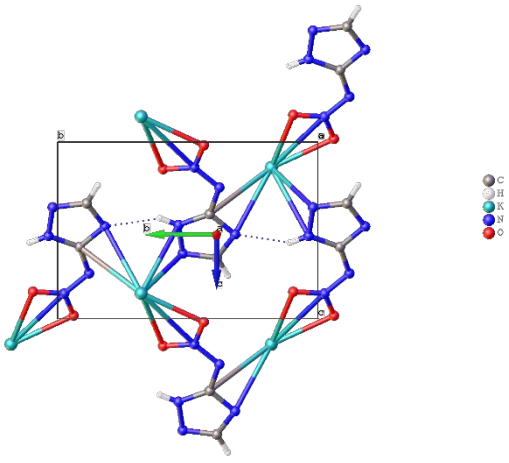


Fig. S16. Packing diagram of compound **11** viewed along the a axis

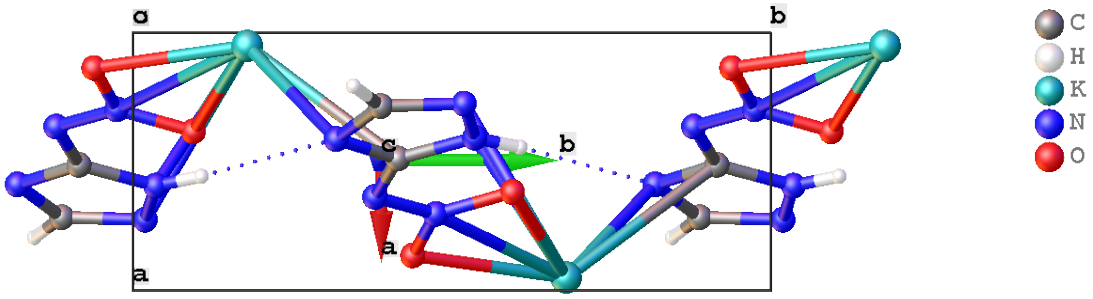


Fig. S17. Packing diagram of compound **11** viewed along the c axis

Table S16: Bond Lengths in Å for compound **11**.

Atom	Atom	Length/Å
K1	O1	2.720(2)
K1	O1[1]	2.788(2)
K1	O2[2]	3.110(3)
K1	O2	2.869(2)
K1	N2[3]	3.232(3)
K1	N2[4]	2.803(3)
K1	N3[5]	3.035(3)
K1	N4[1]	2.855(3)
K1	N4[5]	3.063(3)
K1	N5	3.197(3)
K1	N5[1]	3.281(3)
K1	C1[5]	3.247(3)
O1	N5	1.268(3)
O2	N5	1.258(4)
N1	N2	1.374(3)
N1	C1	1.345(4)
N2	C2	1.318(5)
N3	C1	1.342(4)
N3	C2	1.353(4)
N4	N5	1.312(4)
N4	C1	1.384(4)

[1]2-x,1/2+y,-z; [2]1+x,+y,+z; [3]+x,+y,-1+z; [4]1+x,+y,-1+z; [5]1-x,1/2+y,-z

Table S17: Bond Angles in ° for compound **11**.

Atom	Atom	Atom	Angle/°
O1	K1	O1[1]	138.31(2)
O1[1]	K1	O2	100.81(7)
O1	K1	O2	46.08(7)
O1[1]	K1	O2[2]	85.06(7)
O1	K1	O2[2]	70.25(6)
O1[1]	K1	N2[3]	125.28(8)
O1	K1	N2[4]	65.46(7)
O1[1]	K1	N2[4]	138.62(7)
O1	K1	N2[3]	81.73(8)
O1	K1	N3[5]	133.36(7)
O1[1]	K1	N3[5]	83.31(7)

Atom	Atom	Atom	Angle/°
O1[1]	K1	N4[1]	45.44(7)
O1	K1	N4[5]	121.00(7)
O1	K1	N4[1]	151.84(7)
O1[1]	K1	N4[5]	67.00(7)
O1[1]	K1	N5[1]	22.26(6)
O1[1]	K1	N5	120.16(7)
O1	K1	N5[1]	153.85(6)
O1	K1	N5	22.97(7)
O1	K1	C1[5]	140.61(7)
O1[1]	K1	C1[5]	64.58(7)
O2	K1	O2[2]	85.76(6)
O2[2]	K1	N2[4]	133.67(7)
O2	K1	N2[4]	73.43(7)
O2	K1	N3[5]	123.68(7)
O2	K1	N4[5]	84.58(7)
O2[2]	K1	N5	76.36(6)
O2	K1	N5[1]	123.05(7)
O2[2]	K1	N5[1]	86.35(6)
O2	K1	N5	23.12(7)
O2	K1	C1[5]	109.67(7)
O2[2]	K1	C1[5]	147.66(7)
N2[3]	K1	O2	127.77(8)
N2[3]	K1	O2[2]	76.25(7)
N2[3]	K1	N2[4]	84.55(7)
N2[3]	K1	N3[5]	88.10(7)
N2[3]	K1	N4[1]	81.32(8)
N2[3]	K1	N4[5]	132.41(8)
N2[3]	K1	N5[1]	104.48(8)
N2[3]	K1	N5	104.70(8)
N2[4]	K1	N5[1]	139.66(7)
N2[3]	K1	C1[5]	111.45(8)
N2[4]	K1	C1[5]	78.63(7)
N3[5]	K1	O2[2]	149.90(7)
N3[5]	K1	N2[4]	68.34(7)
N3[5]	K1	N4[5]	45.13(7)
N3[5]	K1	N5[1]	72.70(7)
N3[5]	K1	N5	133.13(7)
N3[5]	K1	C1[5]	24.37(7)
N4[5]	K1	O2[2]	148.00(7)
N4[1]	K1	O2	145.40(7)
N4[1]	K1	O2[2]	83.96(7)
N4[1]	K1	N2[4]	134.51(7)
N45	K1	N24	71.65(8)
N41	K1	N35	68.18(7)
N41	K1	N45	86.89(8)
N41	K1	N5	157.16(7)
N41	K1	N51	23.40(7)
N45	K1	N51	73.74(7)
N45	K1	N5	103.71(7)
N41	K1	C15	67.09(8)
N45	K1	C15	25.12(7)
N5	K1	N24	68.33(7)
N5	K1	N51	141.18(4)

Atom	Atom	Atom	Angle/°
N5	K1	C15	127.64(7)
C15	K1	N51	61.35(7)
K1	O1	K16	154.46(8)
N5	O1	K16	101.32(17)
N5	O1	K1	100.16(18)
K1	O2	K17	85.76(6)
N5	O2	K17	115.51(18)
N5	O2	K1	93.24(17)
N2	N1	K18	72.55(16)
C1	N1	K18	118.41(19)
C1	N1	N2	109.3(3)
K19	N2	K18	84.55(7)
N1	N2	K18	83.52(18)
N1	N2	K19	136.8(2)
C2	N2	K18	116.0(2)
C2	N2	K19	120.2(2)
C2	N2	N1	102.3(3)
C1	N3	K110	86.71(17)
C1	N3	C2	102.5(3)
C2	N3	K110	130.1(2)
K16	N4	K110	86.90(8)
N5	N4	K110	125.60(18)
N5	N4	K16	96.85(17)
N5	N4	C1	117.5(3)
C1	N4	K16	142.5(2)
C1	N4	K110	84.89(17)
K1	N5	K16	112.01(7)
O1	N5	K1	56.86(15)
O1	N5	K16	56.41(15)
O1	N5	N4	115.3(3)
O2	N5	K1	63.63(15)
O2	N5	K16	170.67(19)
O2	N5	O1	120.4(3)
O2	N5	N4	124.3(3)
N4	N5	K1	171.63(19)
N4	N5	K16	59.75(15)
N1	C1	K110	133.6(2)
N1	C1	N4	131.6(3)
N3	C1	K110	68.93(17)
N3	C1	N1	110.1(3)
N3	C1	N4	118.3(3)
N4	C1	K110	69.99(16)
N2	C2	N3	115.7(3)

[1]2-x,1/2+y,-z; [2]1+x,+y,+z; [3]1+x,+y,-1+z; [4]+x,+y,-1+z; [5]1-x,1/2+y,-z; [6]2-x,-1/2+y,-z; [7]-1+x,+y,+z; [8]+x,+y,1+z; [9]-1+x,+y,1+z; [10]1-x,-1/2+y,-z

Table S18: Hydrogen Bond information for compound **11**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
N1	H1	O2	0.79(6)	2.23(5)	2.624(4)	111(4)
N1	H1	N3[1]	0.79(6)	2.20(6)	2.924(4)	153(5)

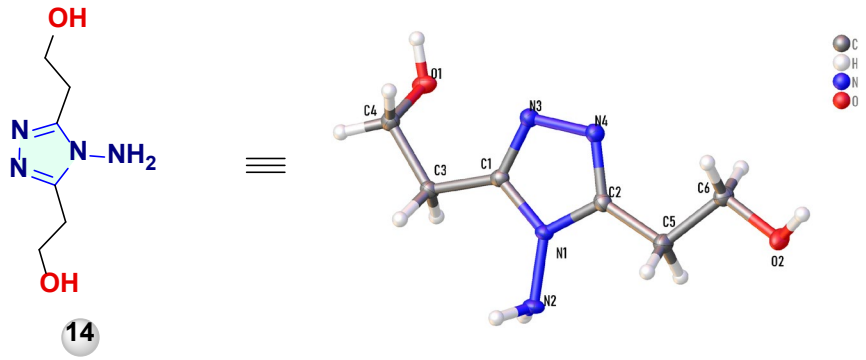
[1]1-x,1/2+y,1-z

Table S19: Torsion Angles in ° for compound **11**.

Atom	Atom	Atom	Atom	Angle/°
K1	O1	N5	K1[1]	-166.10(13)
K1[1]	O1	N5	K1	166.10(13)
K1	O1	N5	O2	3.5(3)
K1[1]	O1	N5	O2	169.6(2)
K1[1]	O1	N5	N4	-10.4(3)
K1	O1	N5	N4	-176.5(2)
K1[2]	O2	N5	K1	86.84(12)
K1	O2	N5	O1	-3.3(3)
K1[2]	O2	N5	O1	83.5(3)
K1	O2	N5	N4	176.8(2)
K1[2]	O2	N5	N4	-96.4(3)
K1[3]	N1	N2	K1[4]	74.9(2)
K1[3]	N1	N2	C2	-115.2(2)
K1[3]	N1	C1	K1[5]	160.16(14)
K1[3]	N1	C1	N3	80.5(3)
K1[3]	N1	C1	N4	-97.5(3)
K1[4]	N2	C2	N3	172.46(19)
K1[3]	N2	C2	N3	-88.3(3)
K1[5]	N3	C1	N1	130.3(2)
K1[5]	N3	C1	N4	-51.4(3)
K1[5]	N3	C2	N2	-96.5(3)
K1[5]	N4	N5	K1[1]	-91.08(18)
K1[5]	N4	N5	O1	-81.0(3)
K1[1]	N4	N5	O1	10.0(2)
K1[5]	N4	N5	O2	98.9(3)
K1[1]	N4	N5	O2	-170.0(2)
K1[1]	N4	C1	K1[5]	-78.1(3)
K1[5]	N4	C1	N1	-131.2(3)
K1[1]	N4	C1	N1	150.7(3)
K1[5]	N4	C1	N3	50.9(3)
K1[1]	N4	C1	N3	-27.2(5)
N1	N2	C2	N3	0.4(4)
N2	N1	C1	K1[5]	80.0(3)
N2	N1	C1	N3	0.4(3)
N2	N1	C1	N4	-177.6(3)
N5	N4	C1	K1[5]	127.8(3)
N5	N4	C1	N1	-3.4(5)
N5	N4	C1	N3	178.7(3)
C1	N1	N2	K1[3]	114.7(2)
C1	N1	N2	K1[4]	-170.4(2)
C1	N1	N2	C2	-0.5(3)
C1	N3	C2	N2	-0.2(4)
C1	N4	N5	K1[1]	164.5(3)
C1	N4	N5	O1	174.5(2)
C1	N4	N5	O2	-5.6(4)
C2	N3	C1	K1[5]	-130.4(2)
C2	N3	C1	N1	-0.1(3)

Atom	Atom	Atom	Atom	Angle/°
C2	N3	C1	N4	178.2(3)

Table S20. Single crystal X-ray data and structure refinement for compound **14**.[6-10]



Formula	$C_6H_{12}N_4O_2$
$D_{calc.}$/ g cm^{-3}	1.428
m/mm^{-1}	0.923
Formula Weight	172.20
Color	colourless
Shape	block-shaped
Size/mm^3	0.24×0.19×0.06
T/K	99.99(10)
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	7.80690(8)
b/Å	5.75687(6)
c/Å	17.86698(18)
a/°	90
b/°	94.2689(9)
g/°	90
V/Å^3	800.773(14)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu K$_a$
Q_{min}/°	4.964
Q_{max}/°	76.992
Measured Refl's.	7110
Indep't Refl's	1607
Refl's I≥2 s(I)	1532
R_{int}	0.0245
Parameters	125
Restraints	0
Largest Peak	0.205
Deepest Hole	-0.266
GooF	1.074
wR_2 (all data)	0.0820
wR_2	0.0812
R_1 (all data)	0.0335
R_1	0.0325

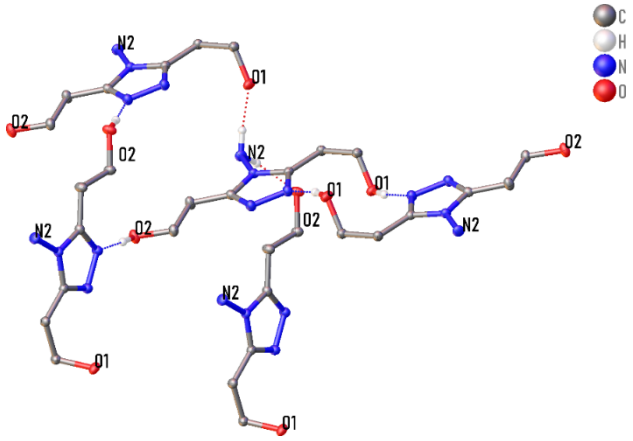


Fig. S18. The following hydrogen bonding interactions with a maximum D-D distance of 3.1 Å and a minimum angle of 110 ° are present in compound **14**: O1–N3_*4: 2.765 Å, O2–N4*_1: 2.769 Å, N2–O1_*2: 2.926 Å, N2–O2*_3: 2.952 Å.

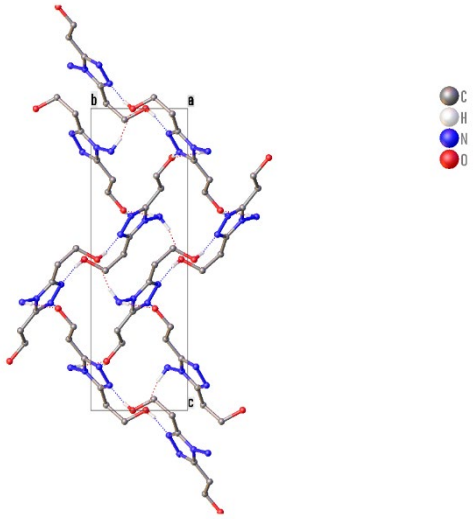


Fig. S19. Packing diagram of compound **14**.

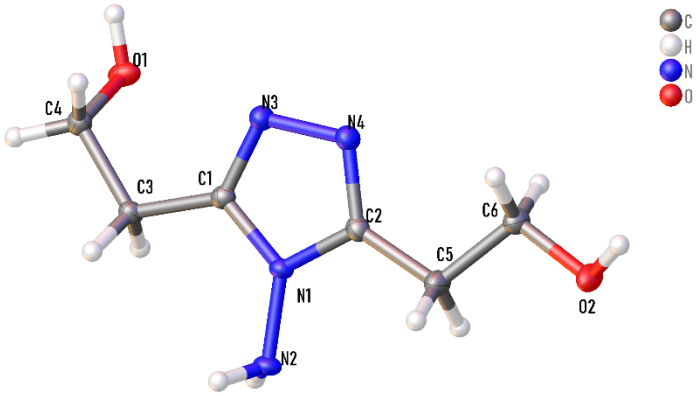


Fig. S20. Molecular structure (thermal ellipsoid plot (50%) of compound **14** (CCDC, 2296316).

Table S21: Bond Lengths in Å for compound **14**.

Atom	Atom	Length/Å
O1	C4	1.4194(13)
O2	C6	1.4241(13)
N1	N2	1.4099(12)
N1	C1	1.3695(14)
N1	C2	1.3621(13)
N3	N4	1.3974(12)
N3	C1	1.3106(14)
N4	C2	1.3086(14)
C1	C3	1.4922(14)
C2	C5	1.4889(15)
C3	C4	1.5181(15)
C5	C6	1.5128(15)

Table S22: Bond Angles in ° for compound **14**.

Atom	Atom	Atom	Angle/°
C1	N1	N2	129.16(9)
C2	N1	N2	124.15(9)
C2	N1	C1	106.63(9)
C1	N3	N4	107.56(9)
C2	N4	N3	107.69(8)
N1	C1	C3	123.12(9)
N3	C1	N1	108.94(9)
N3	C1	C3	127.94(10)
N1	C2	C5	123.45(9)
N4	C2	N1	109.18(9)
N4	C2	C5	127.36(10)
C1	C3	C4	113.45(9)
O1	C4	C3	110.09(9)
C2	C5	C6	111.95(9)
O2	C6	C5	108.78(9)

Table S23: Torsion Angles in ° for compound **14**.

Atom	Atom	Atom	Atom	Angle/°
N1	C1	C3	C4	-179.37(9)
N1	C2	C5	C6	174.30(10)
N2	N1	C1	N3	177.12(10)
N2	N1	C1	C3	-2.67(17)
N2	N1	C2	N4	-177.30(9)
N2	N1	C2	C5	1.41(16)
N3	N4	C2	N1	-0.02(12)
N3	N4	C2	C5	-178.67(10)
N3	C1	C3	C4	0.88(16)
N4	N3	C1	N1	0.02(12)
N4	N3	C1	C3	179.80(10)
N4	C2	C5	C6	-7.23(16)
C1	N1	C2	N4	0.03(12)
C1	N1	C2	C5	178.74(10)
C1	N3	N4	C2	0.00(12)
C1	C3	C4	O1	70.24(12)
C2	N1	C1	N3	-0.03(12)
C2	N1	C1	C3	-179.83(10)
C2	C5	C6	O2	179.65(9)

Table S24: Hydrogen Bond information for compound **14**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/deg
O1	H1	N3[1]	0.881(19)	1.891(19)	2.7653(12)	171.3(17)
O2	H2	N4[2]	0.869(19)	1.901(19)	2.7686(12)	176.9(16)
N2	H2A	O2[3]	0.909(16)	2.068(16)	2.9519(13)	163.8(14)
N2	H2B	O1[4]	0.906(17)	2.116(16)	2.9264(13)	148.5(14)

[1]1-x,2-y,1-z; [2]3/2-x,-1/2+y,1/2-z; [3]1/2-x,1/2+y,1/2-z; [4]+x,-1+y,+z

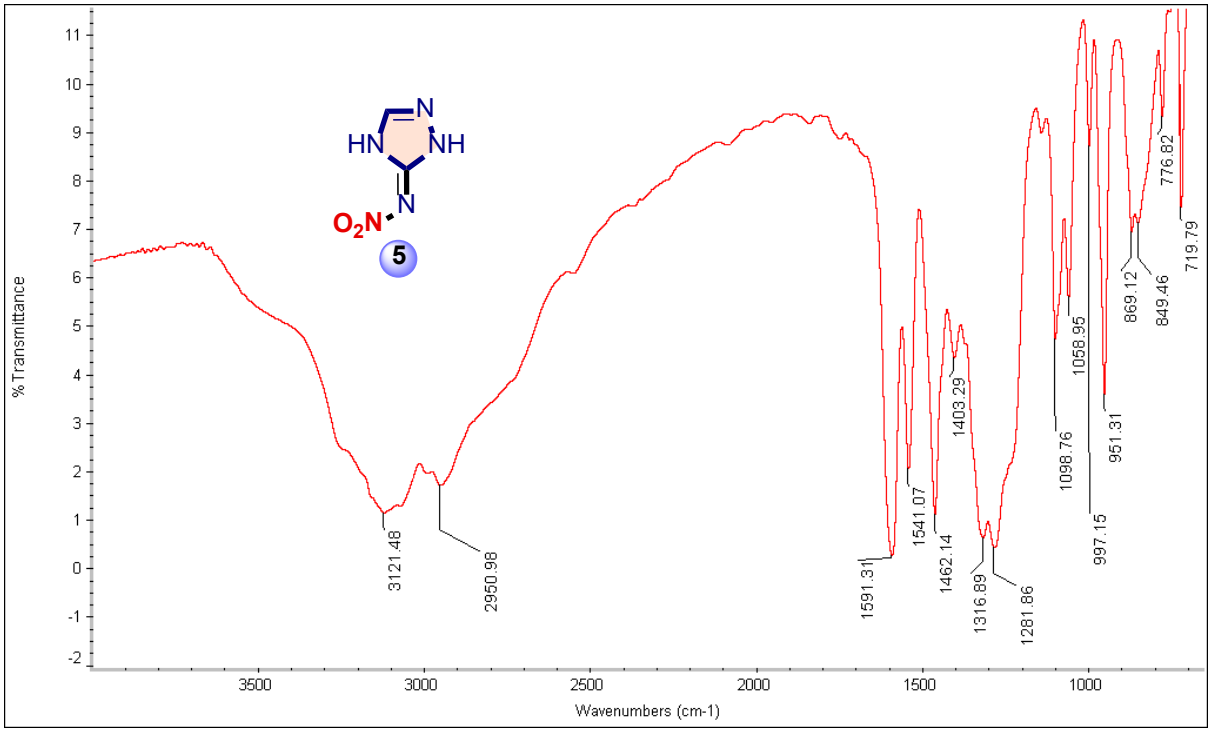


Fig. S21. FTIR-Spectrum of Compound **5**.

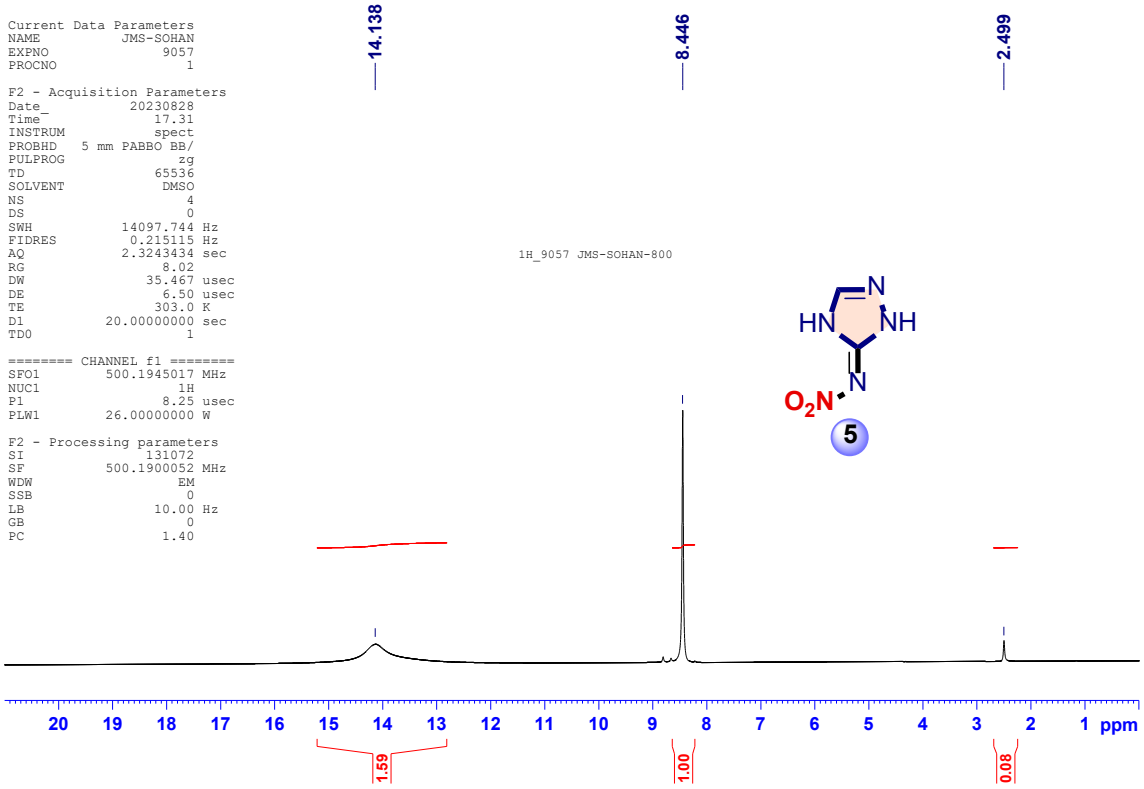


Fig. S22. ^{1}H NMR Spectrum of Compound **5** (500.19 MHz).

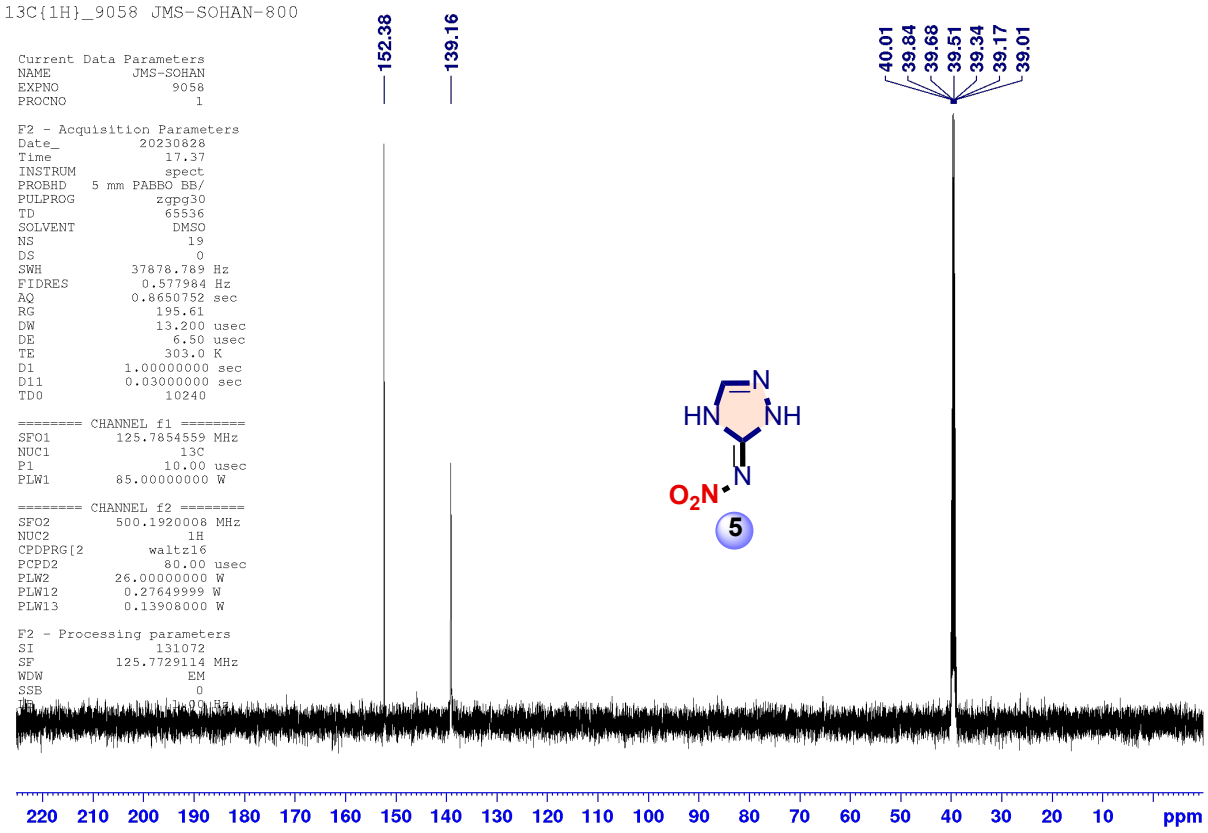


Fig. S23. ^{13}C NMR Spectrum of Compound **5** (125.77 MHz).

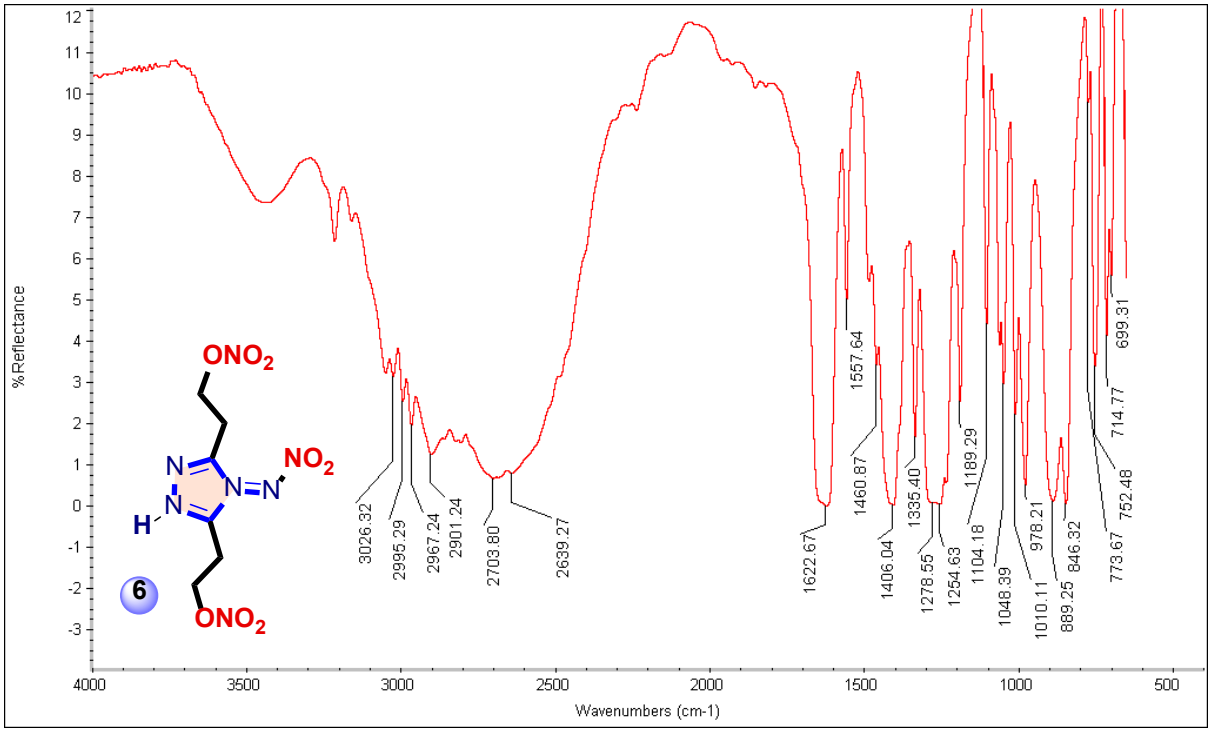


Fig. S24. FTIR-Spectrum of Compound **6**.

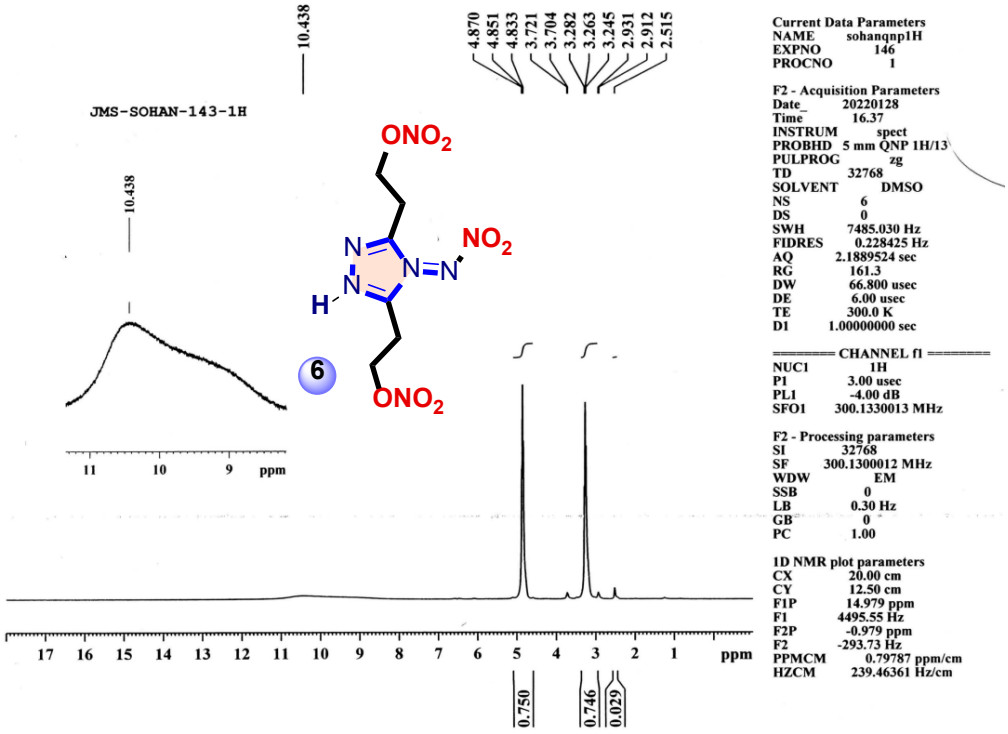


Fig. S25. ^{1}H NMR Spectrum of Compound **6** (300.13 MHz).

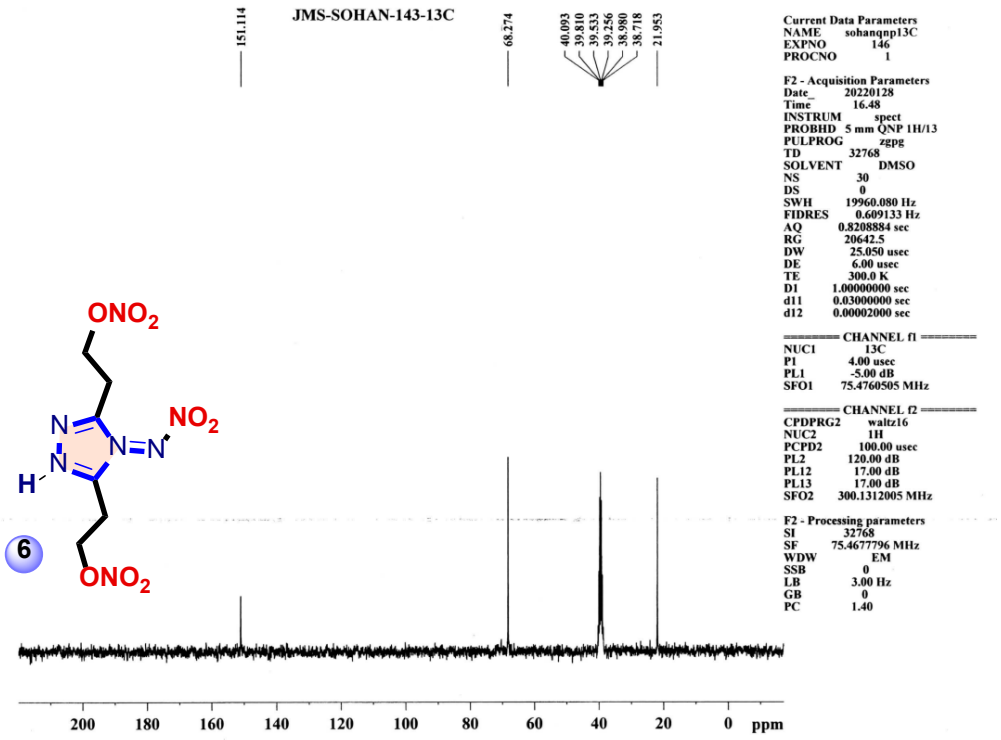


Fig. S26. ^{13}C NMR Spectrum of Compound **6** (100.00 MHz).

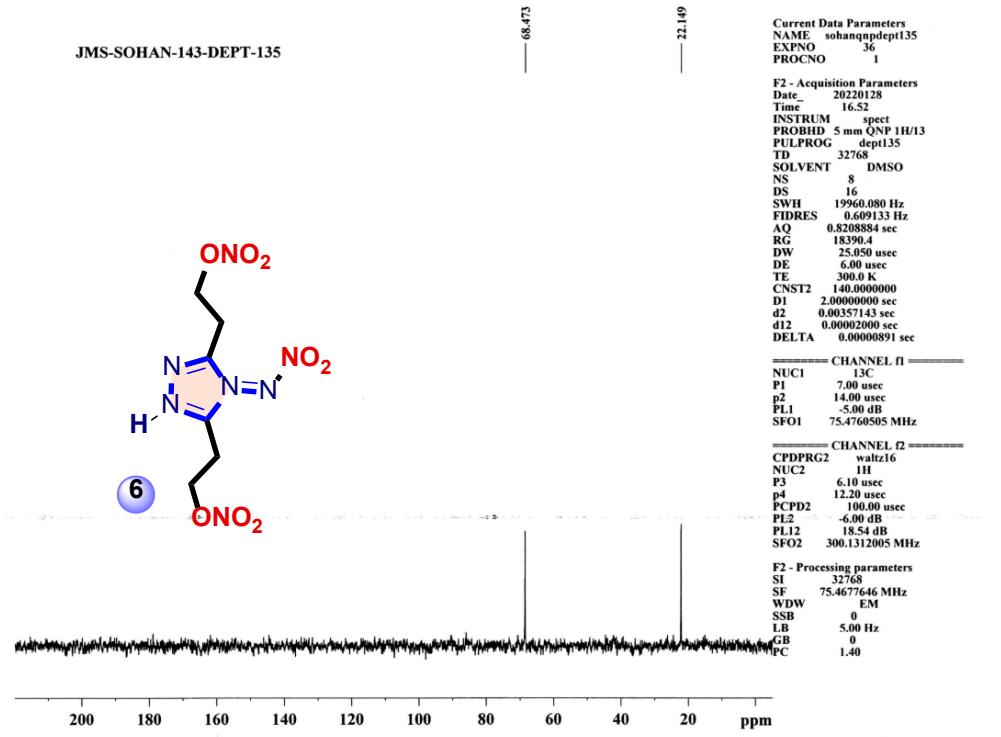


Fig. S27. ^{13}C-DEPT NMR Spectrum of Compound **6** (100.00 MHz).

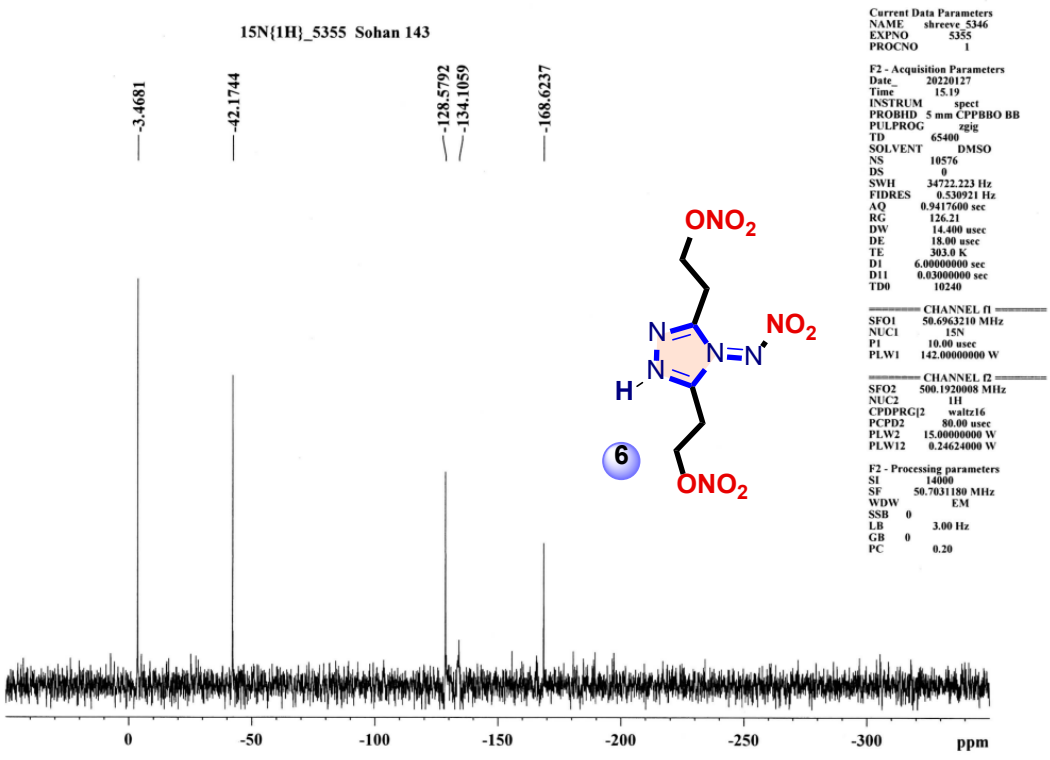


Fig. S28. ^{1}H NMR Spectrum of Compound **6** (500.19 MHz).

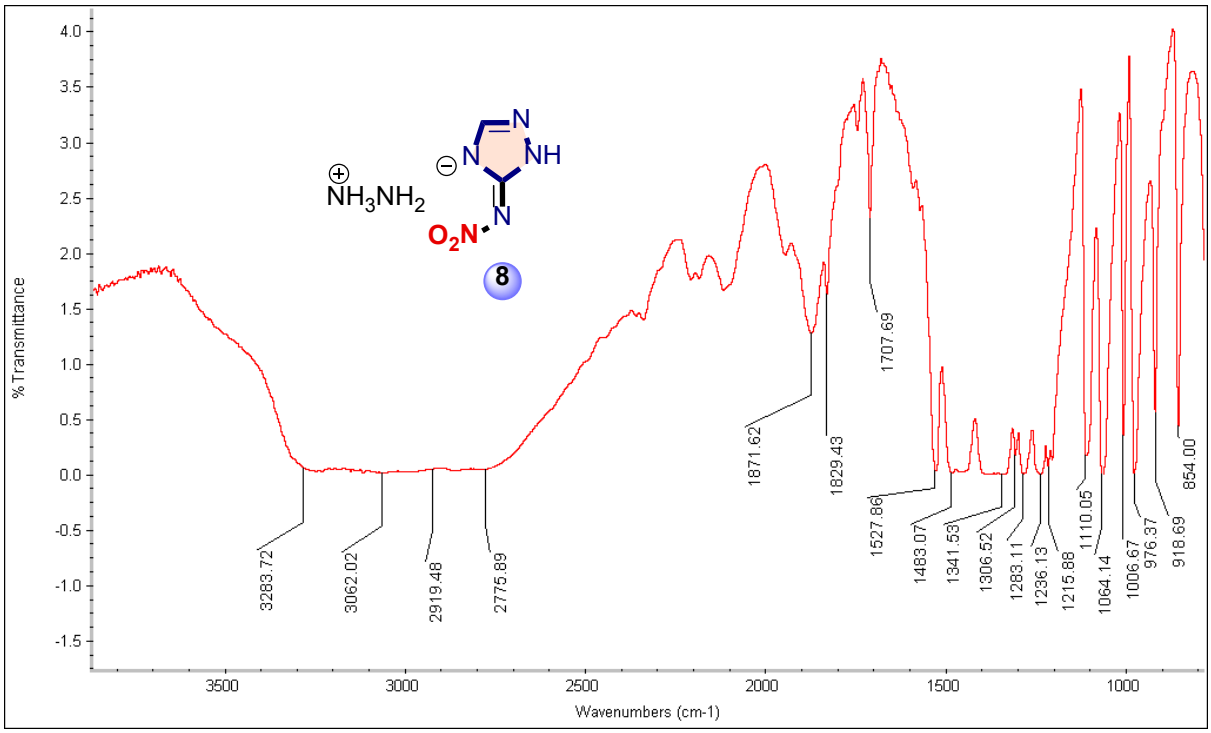


Fig. S29. FTIR-Spectrum of Compound **8**.

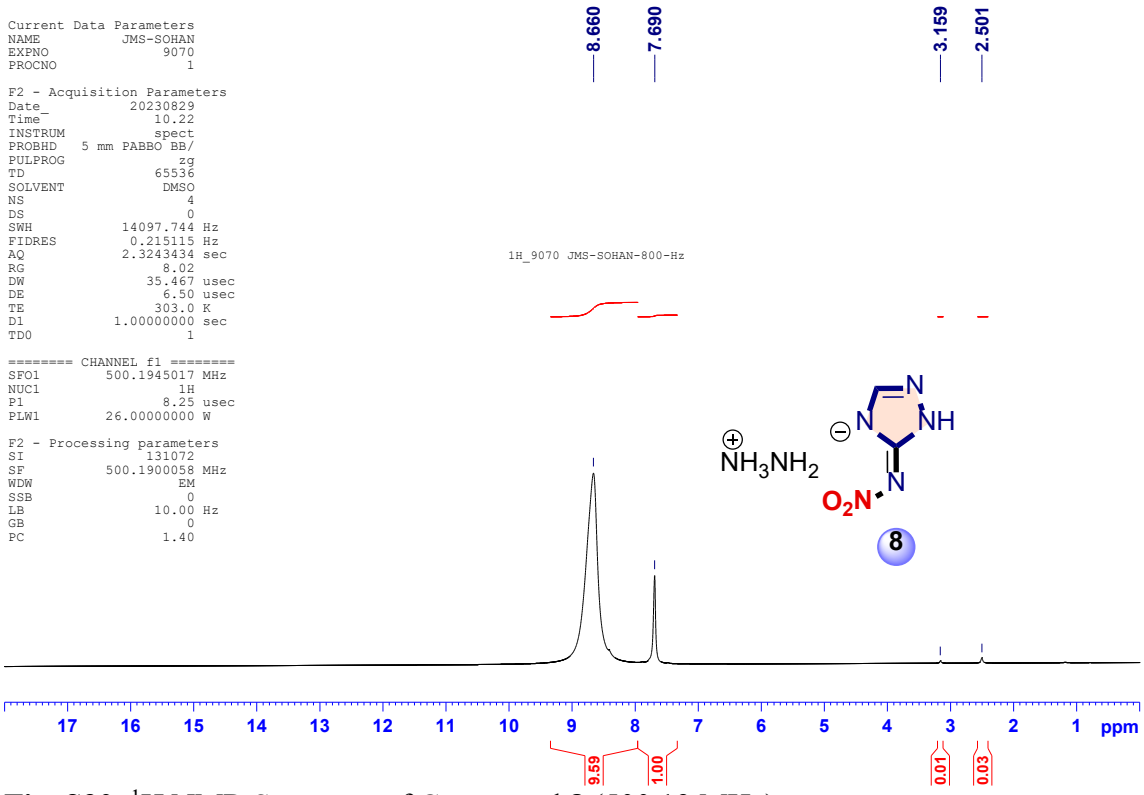


Fig. S30. ^{1}H NMR Spectrum of Compound **8** (500.19 MHz).

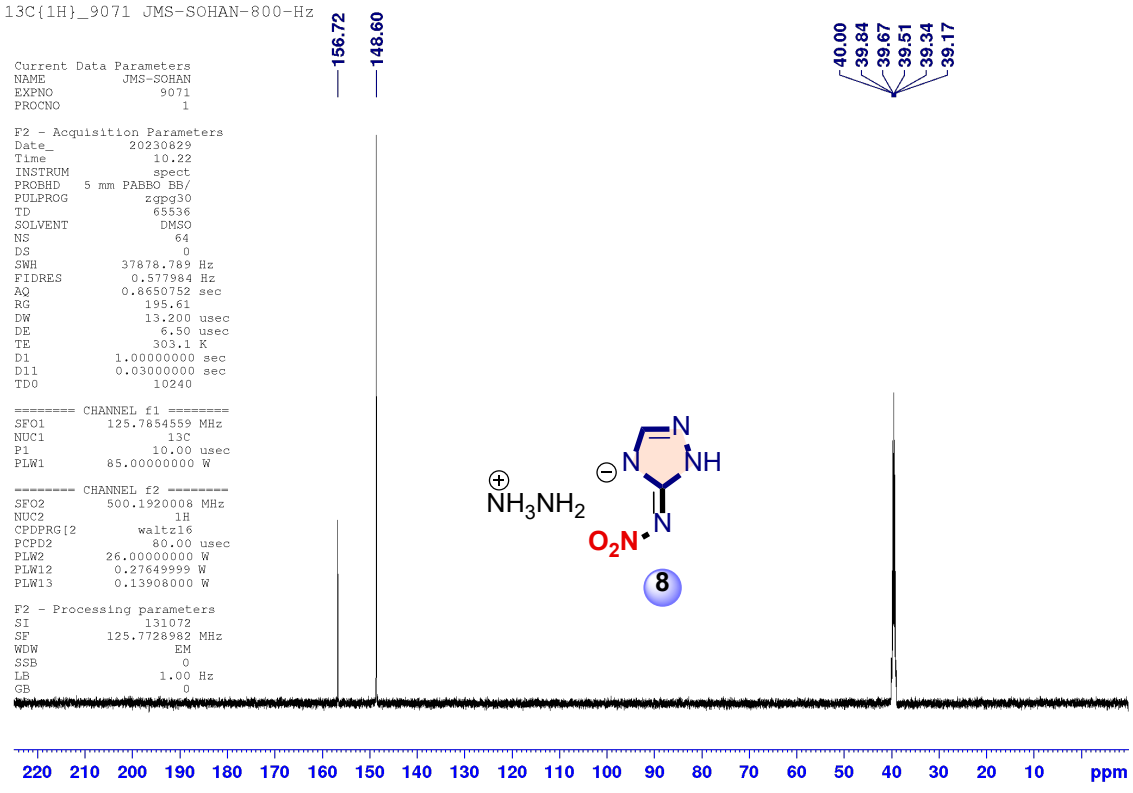


Fig. S31. ^{13}C NMR Spectrum of Compound **8** (125.77 MHz).

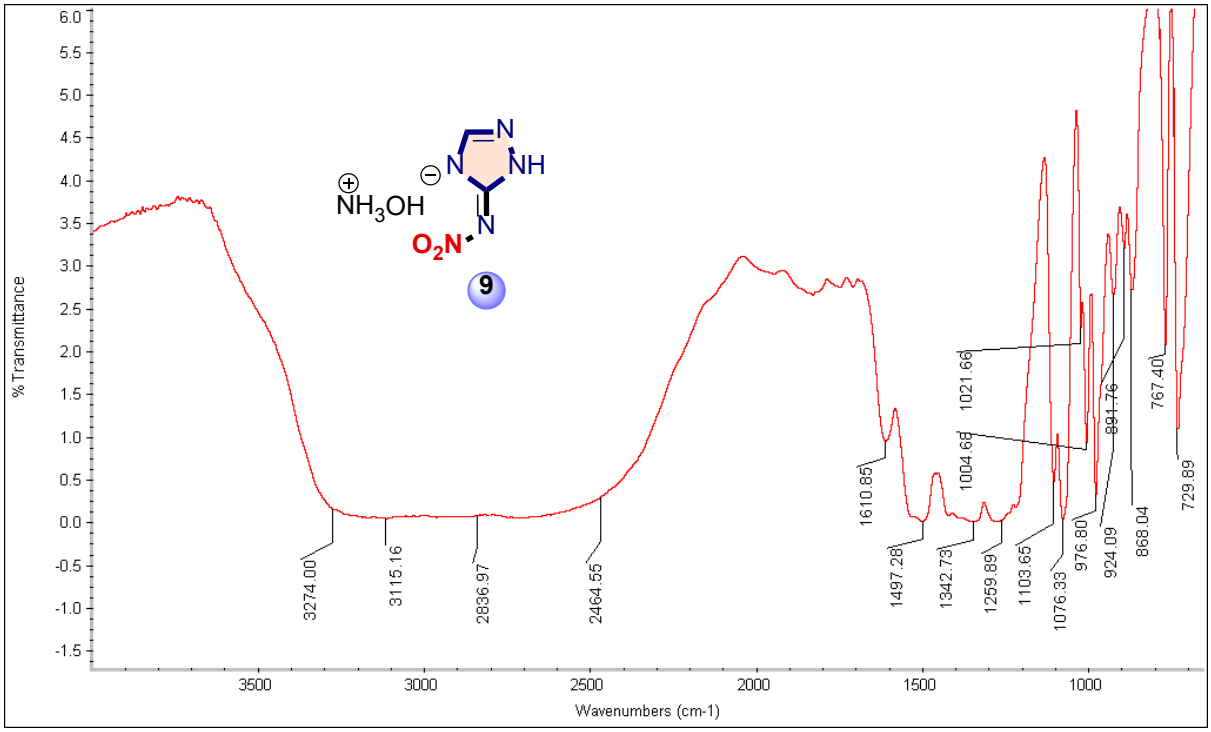


Fig. S32. FTIR-Spectrum of Compound **9**.

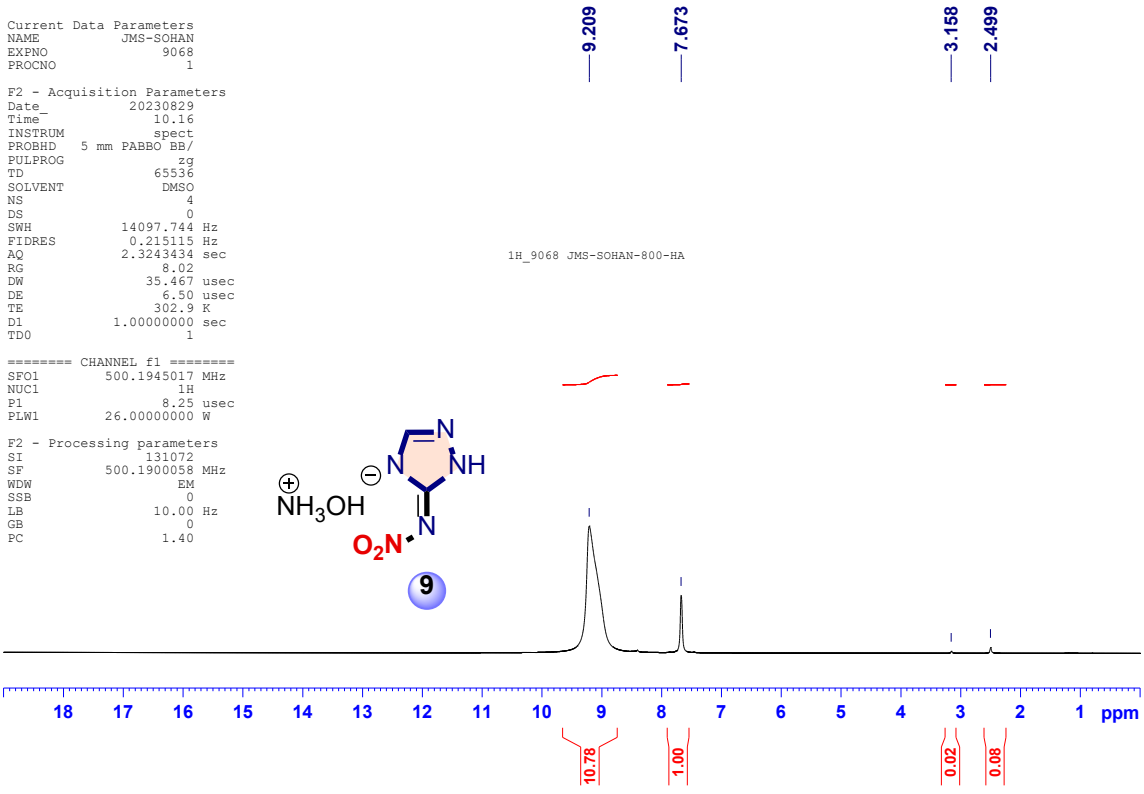


Fig. S33. ^{1}H NMR Spectrum of Compound **9** (500.19 MHz).

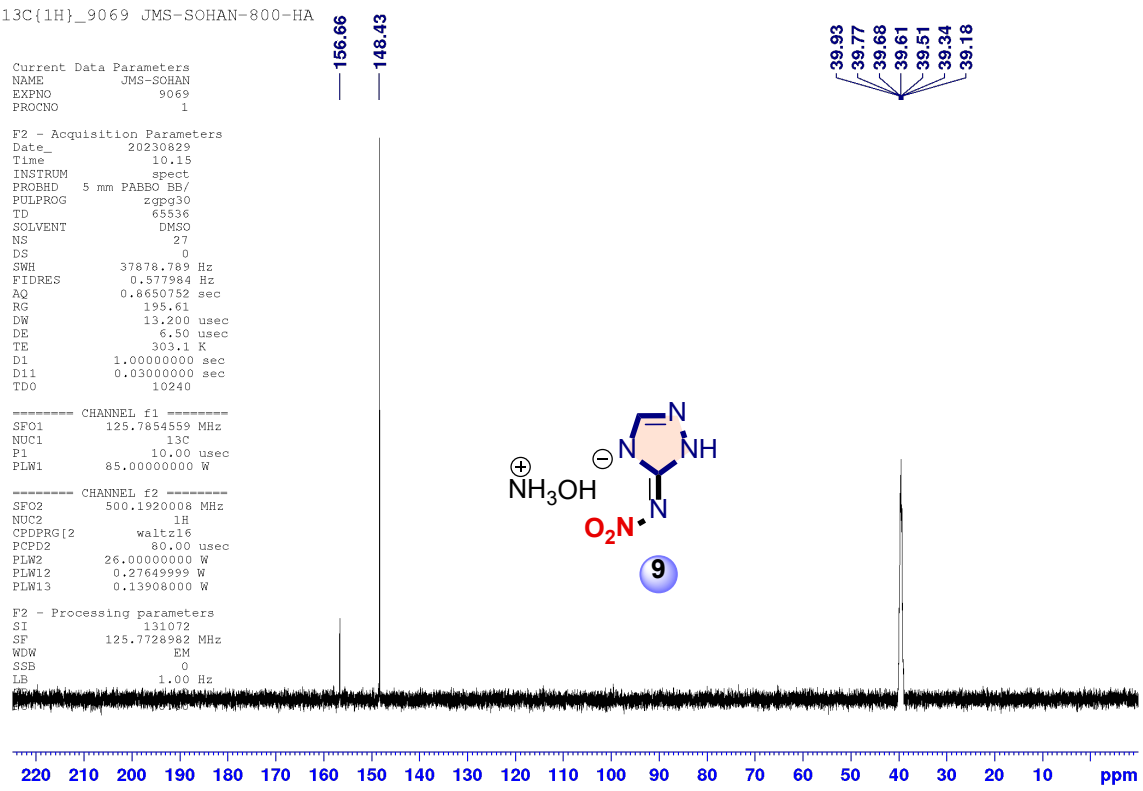


Fig. S34. ^{13}C NMR Spectrum of Compound **9** (125.77 MHz).

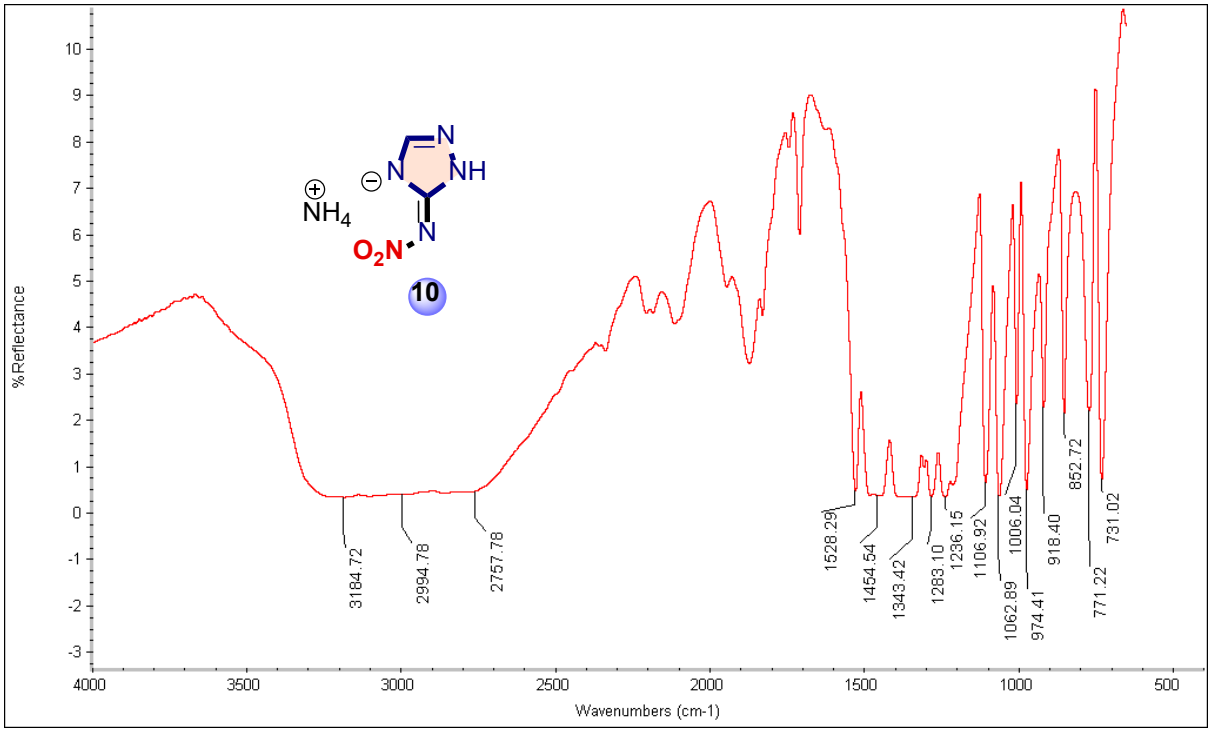


Fig. S35. FTIR-Spectrum of Compound **10**.

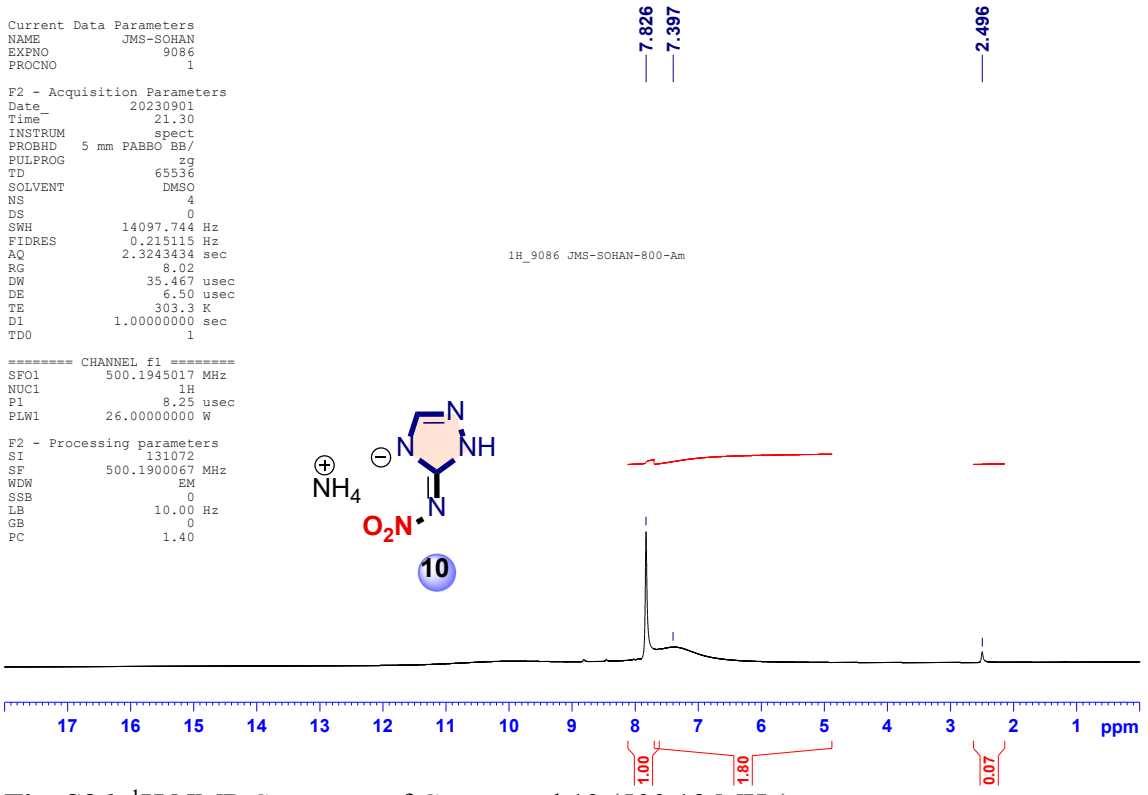


Fig. S36. ^{1}H NMR Spectrum of Compound **10** (500.19 MHz).

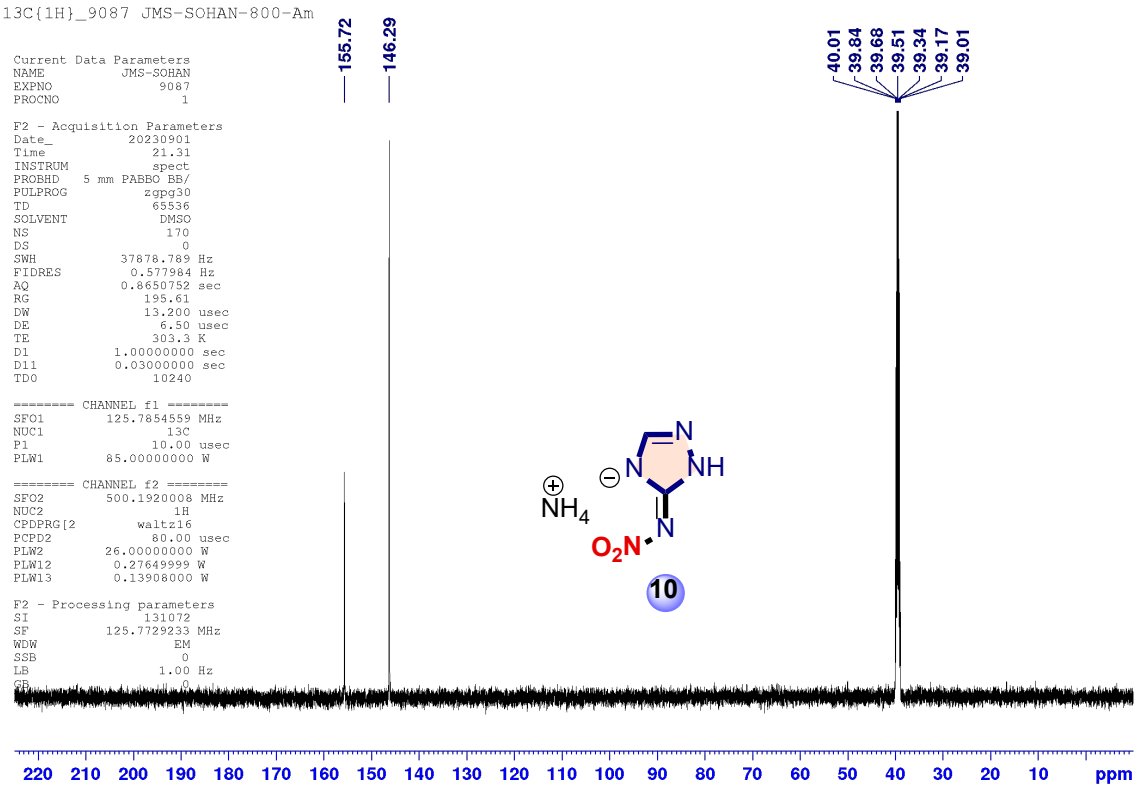


Fig. S37. ^{13}C NMR Spectrum of Compound **10** (125.77 MHz).

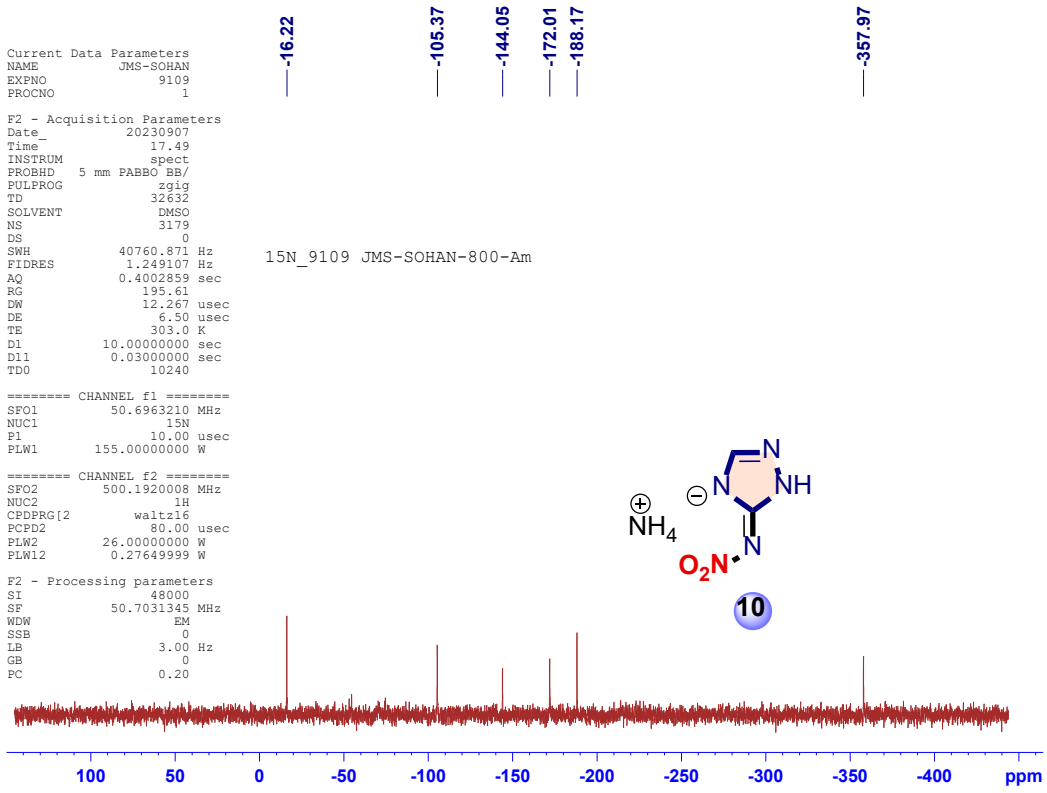


Fig. S38. ^{1}H NMR Spectrum of Compound **10** (500.19 MHz).

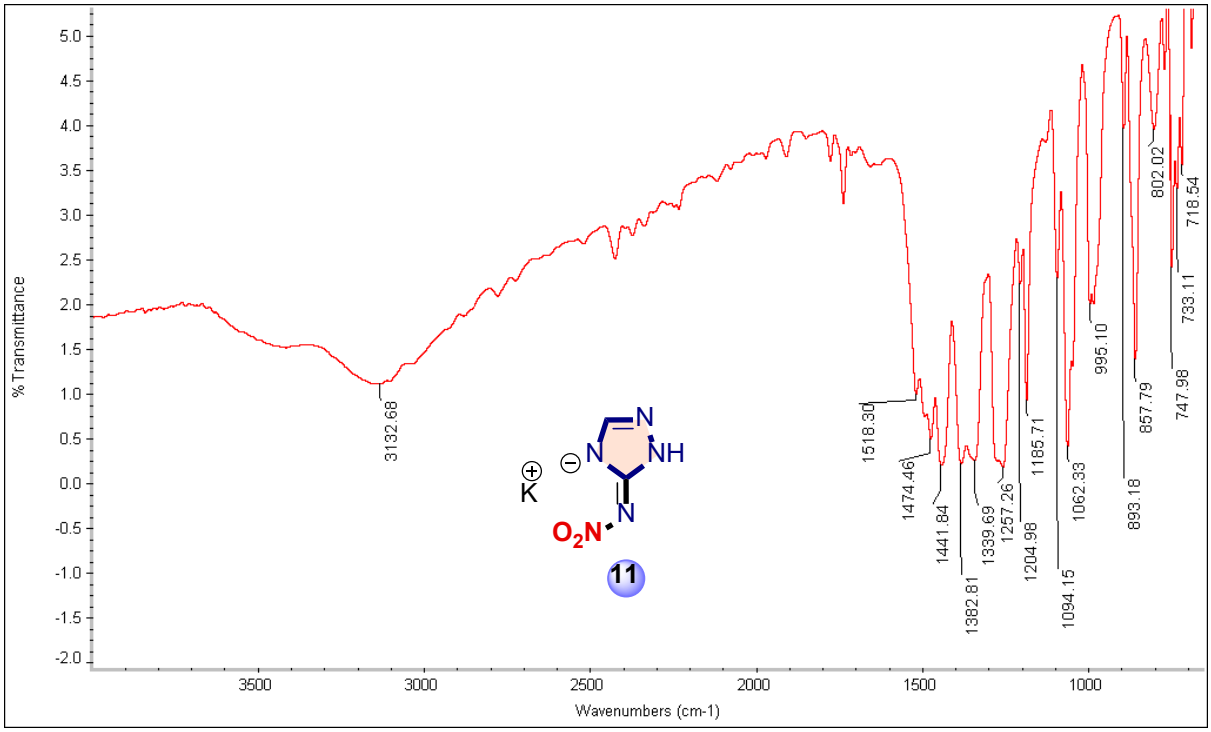


Fig. S39. FTIR-Spectrum of Compound **11**.

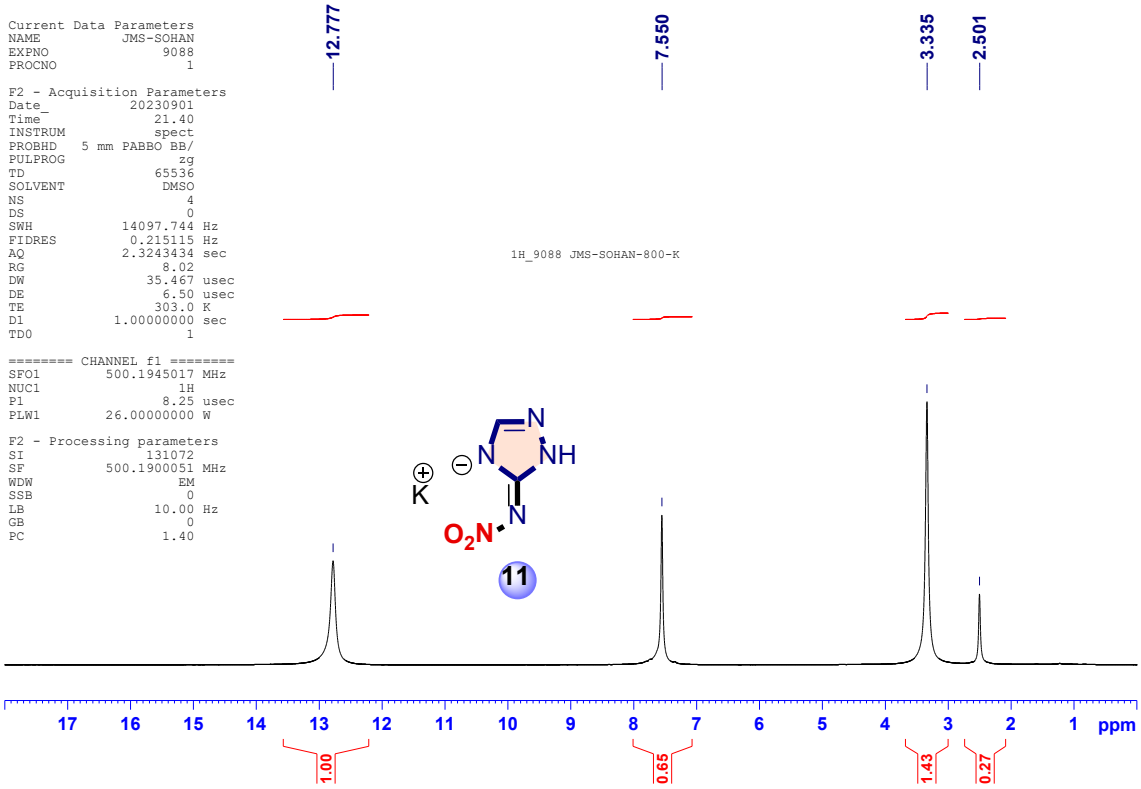


Fig. S40. [1]H NMR Spectrum of Compound **11** (500.19 MHz).

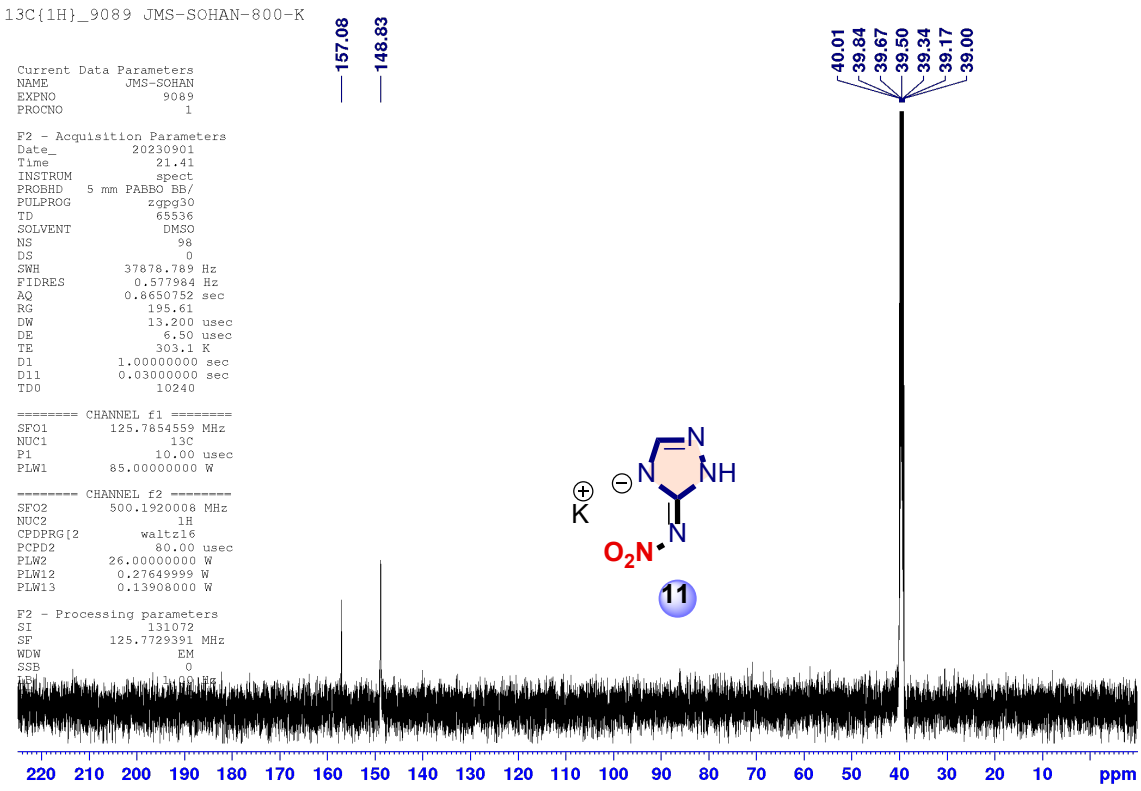


Fig. S41. [13]C NMR Spectrum of Compound **11** (125.77 MHz).

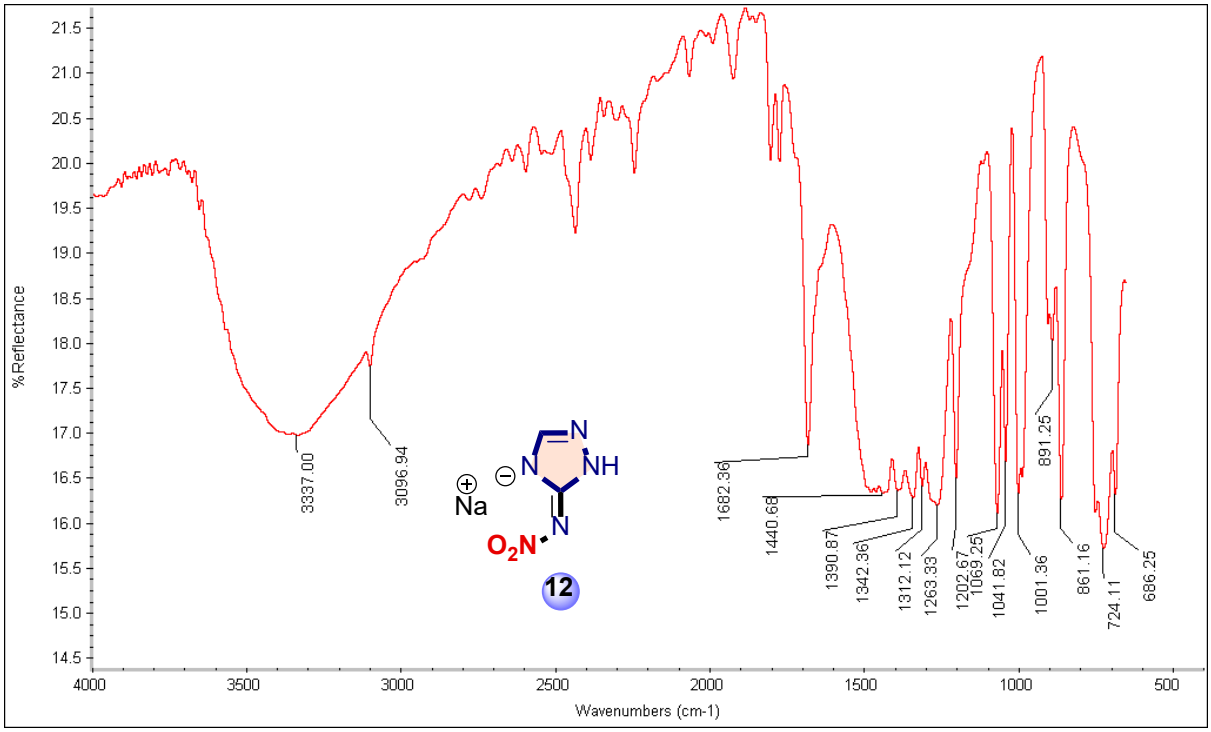


Fig. S42. FTIR-Spectrum of Compound **12**.

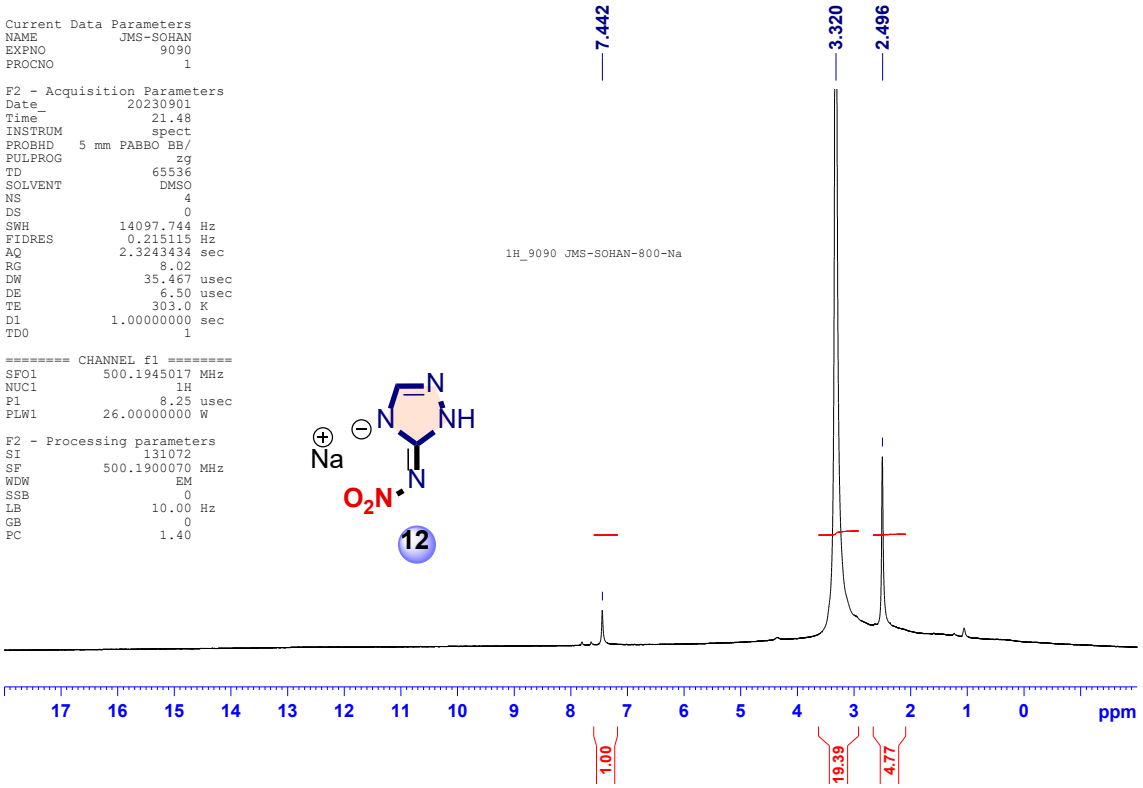


Fig. S43. ^{1}H NMR Spectrum of Compound **12** (500.19 MHz).

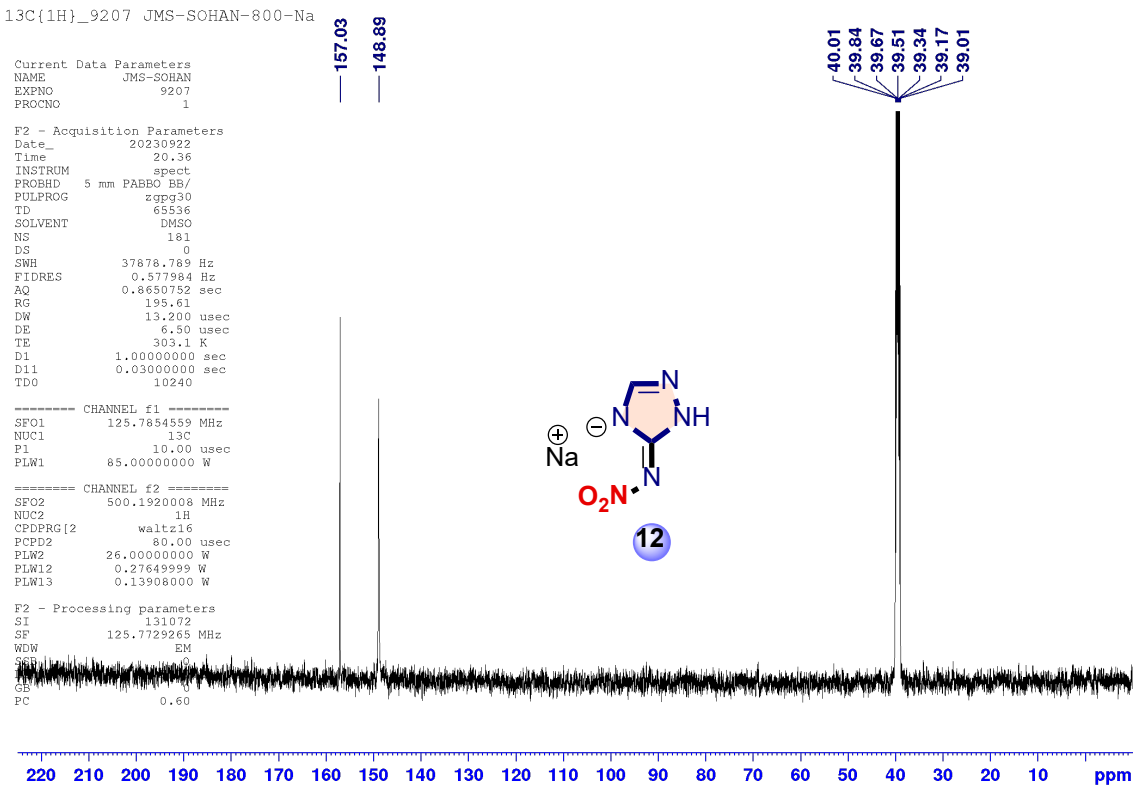


Fig. S44. ^{13}C NMR Spectrum of Compound **12** (125.77 MHz).

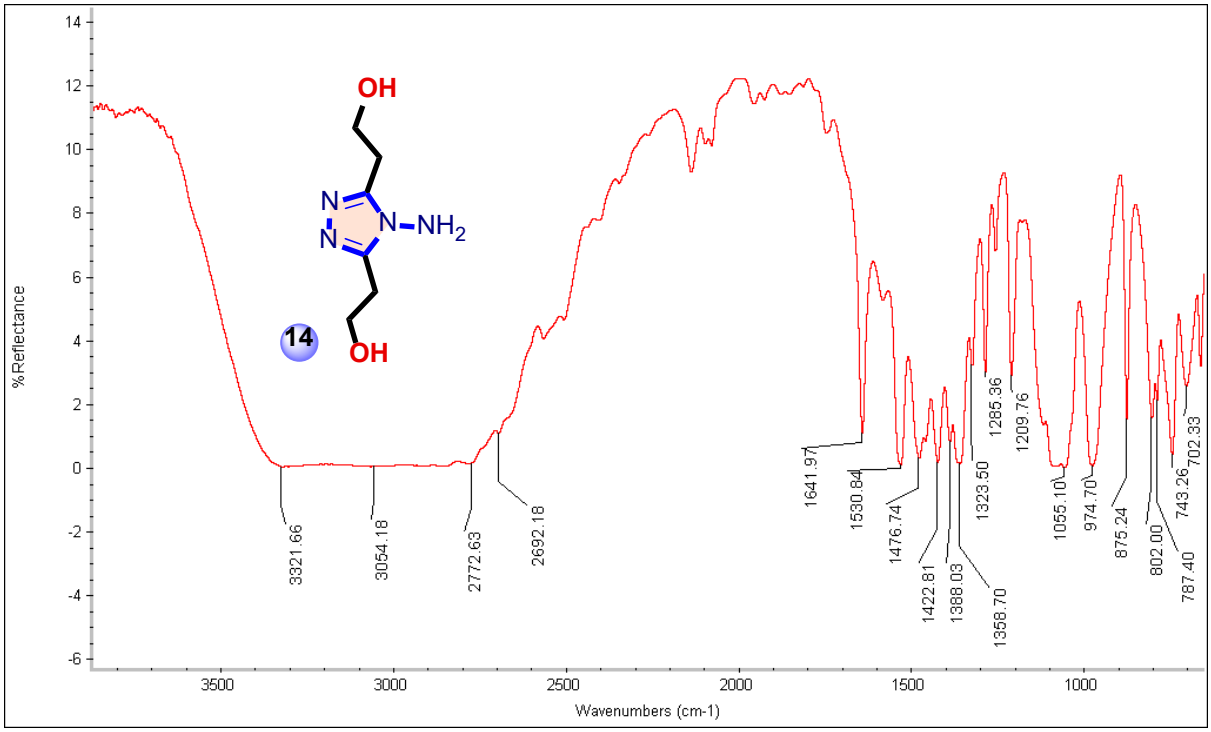


Fig. S45. FTIR-Spectrum of Compound **14**.

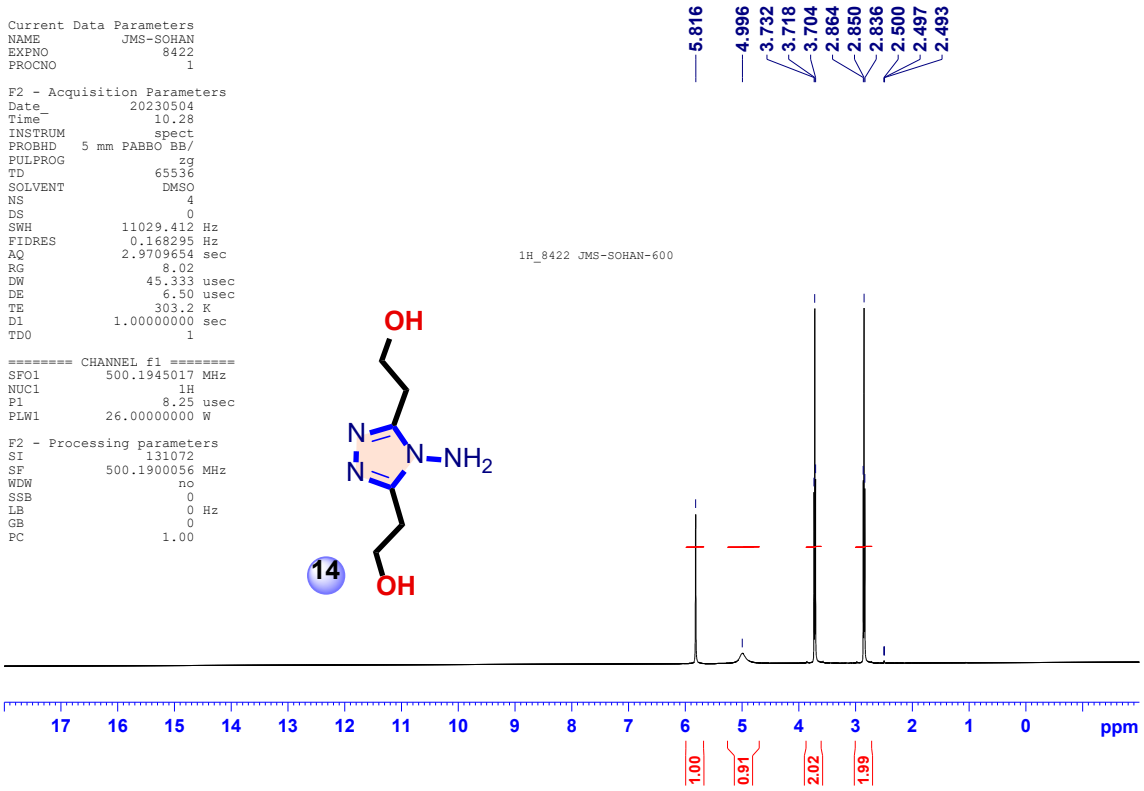


Fig. S46. ^{1}H NMR Spectrum of Compound **14** (500.19 MHz).

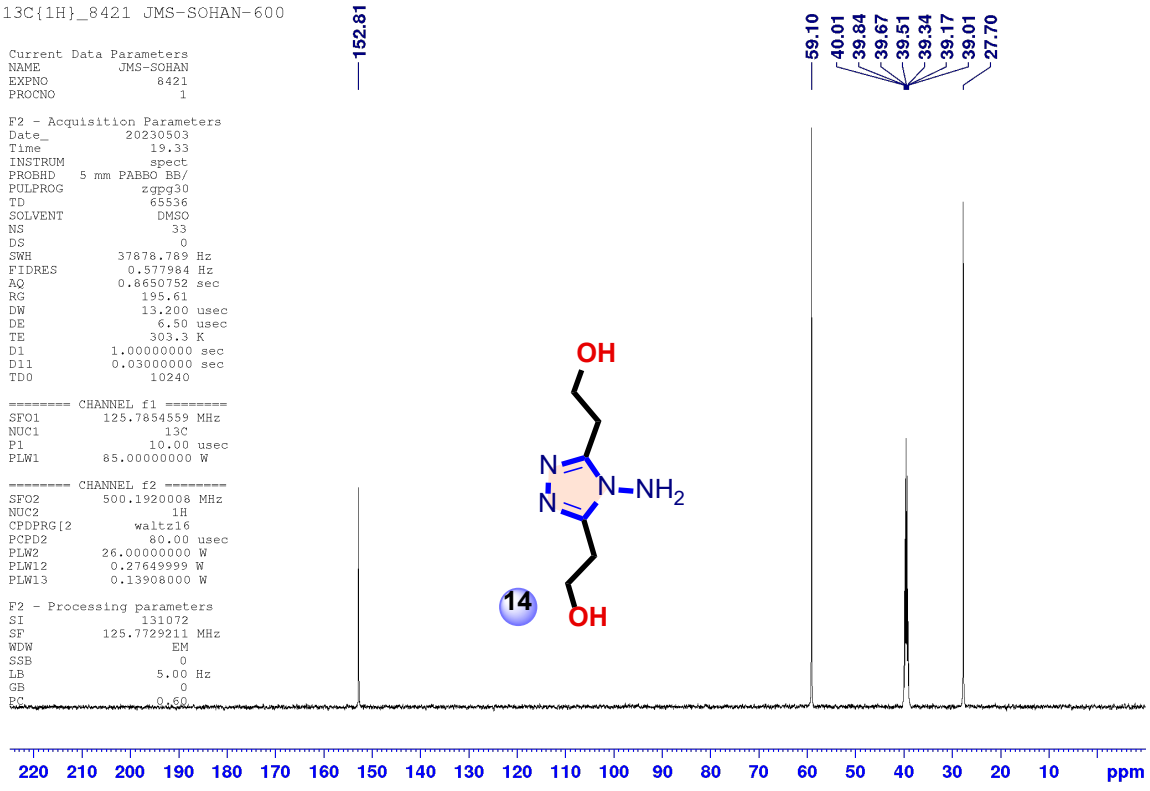


Fig. S47. ^{13}C NMR Spectrum of Compound **14** (125.77 MHz).

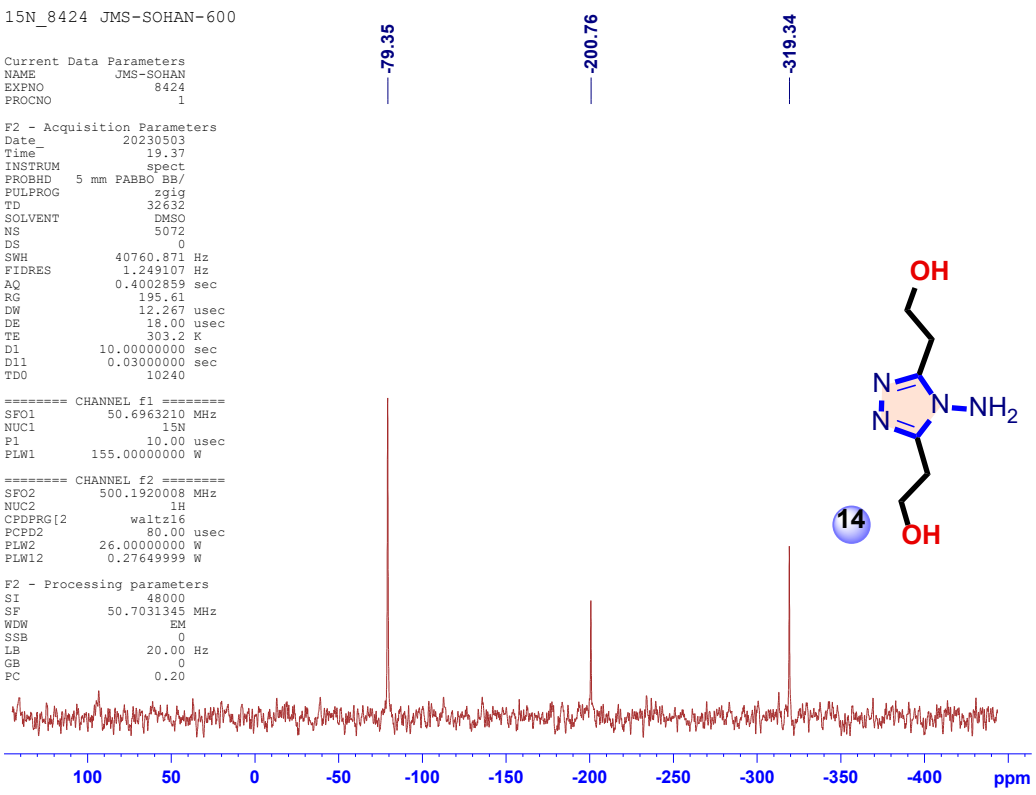


Fig. S48. ^{1}H NMR Spectrum of Compound **14** (500.19 MHz).

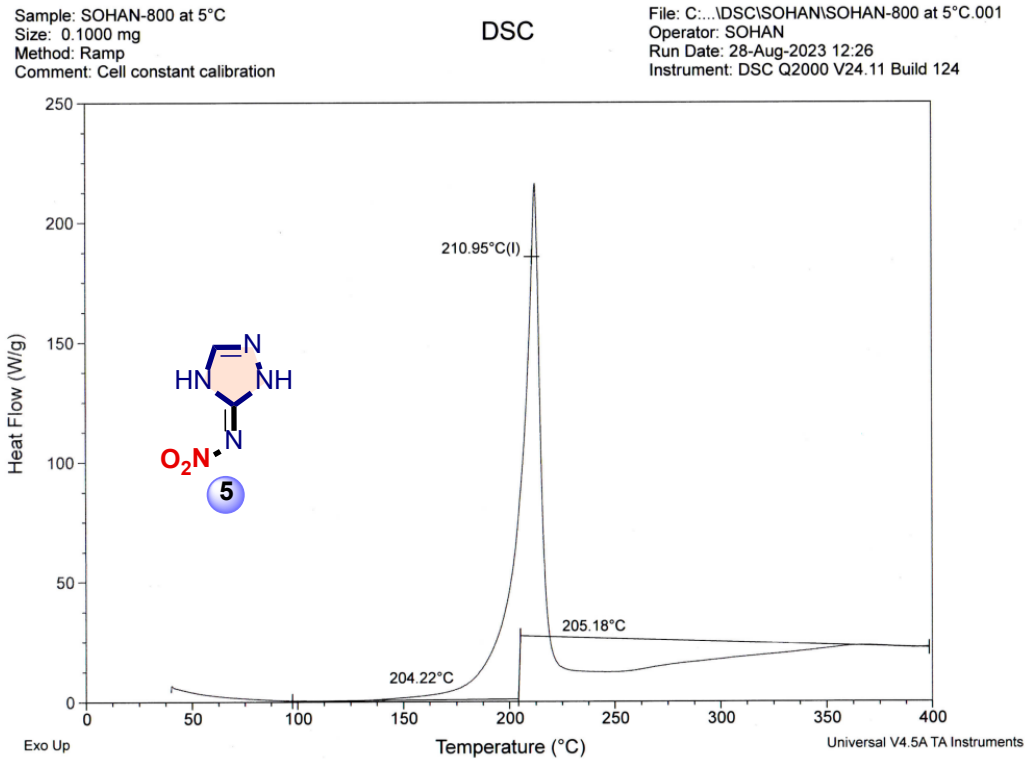


Fig. S49. DSC of compound **5** at 5 °C min^{-1}

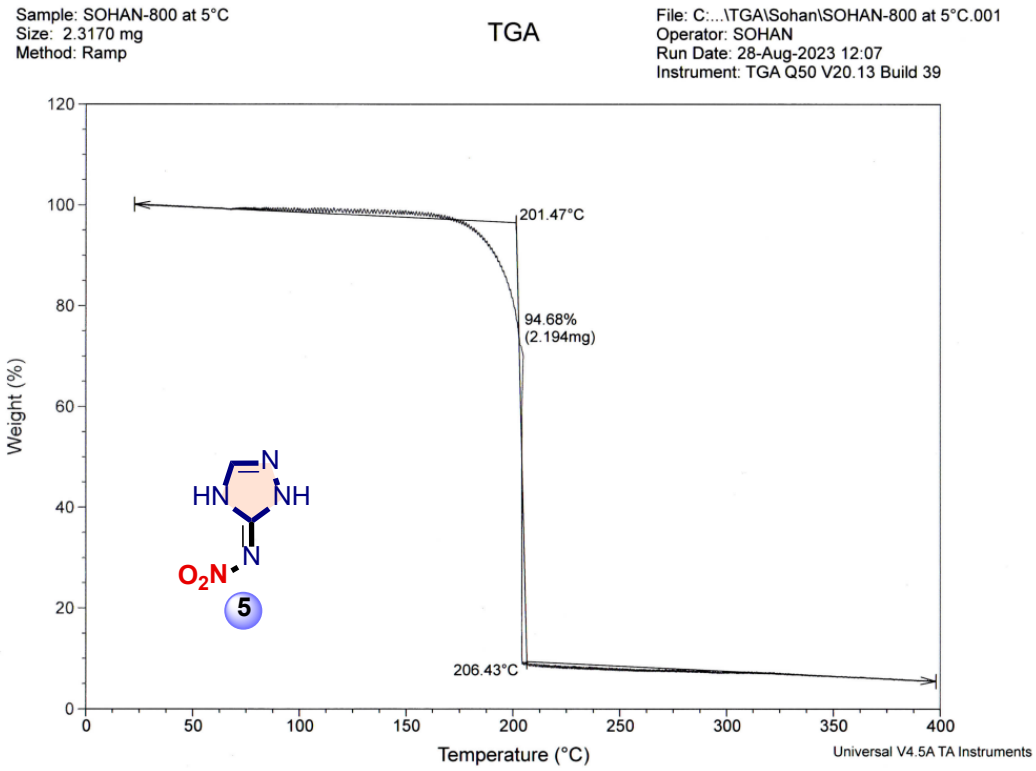


Fig. S50. TGA of compound **5** at 5 °C min^{-1}

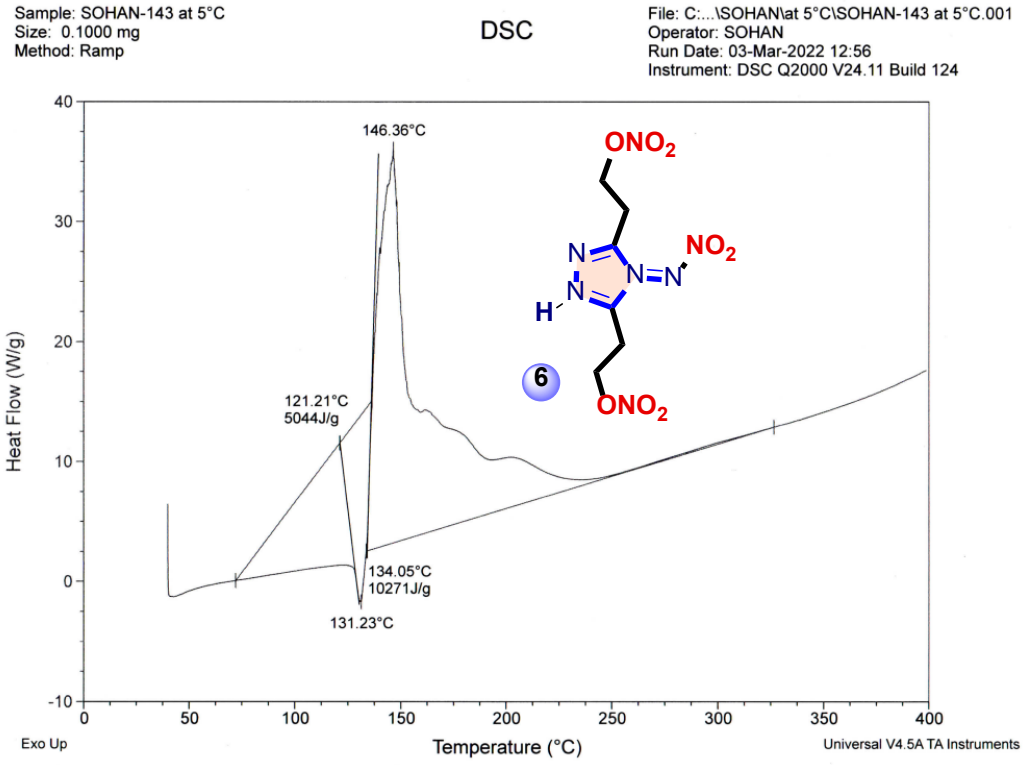


Fig. S51. DSC of compound **6** at 5 °C min^{-1}

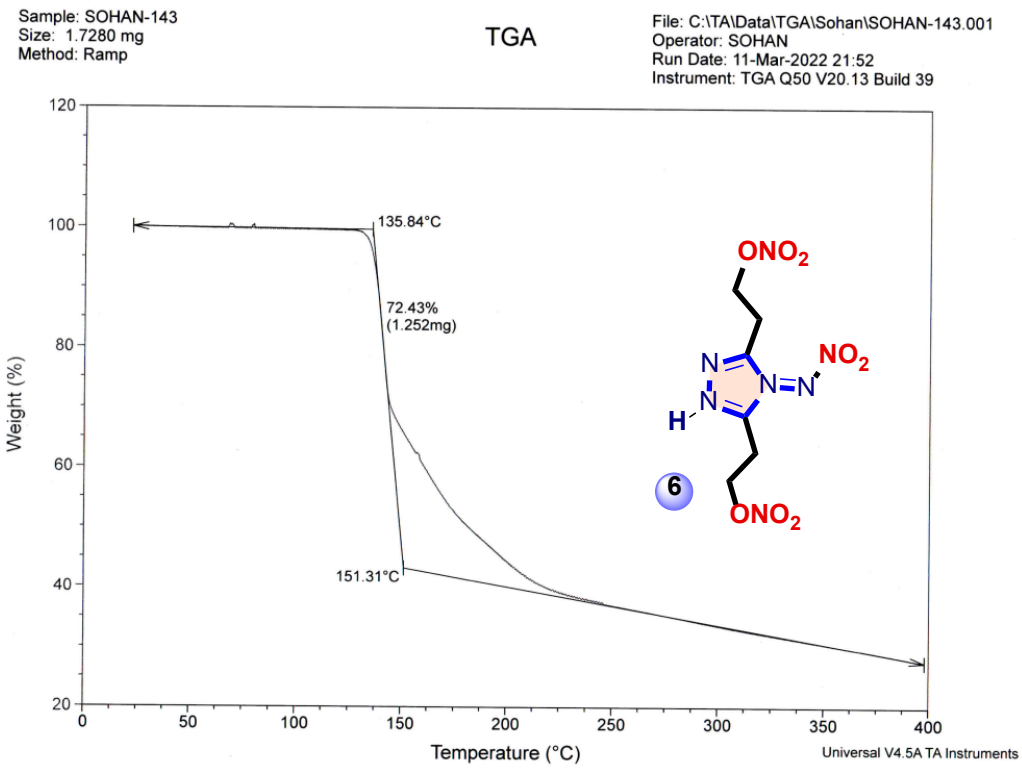


Fig. S52. TGA of compound **6** at 5 °C min^{-1}

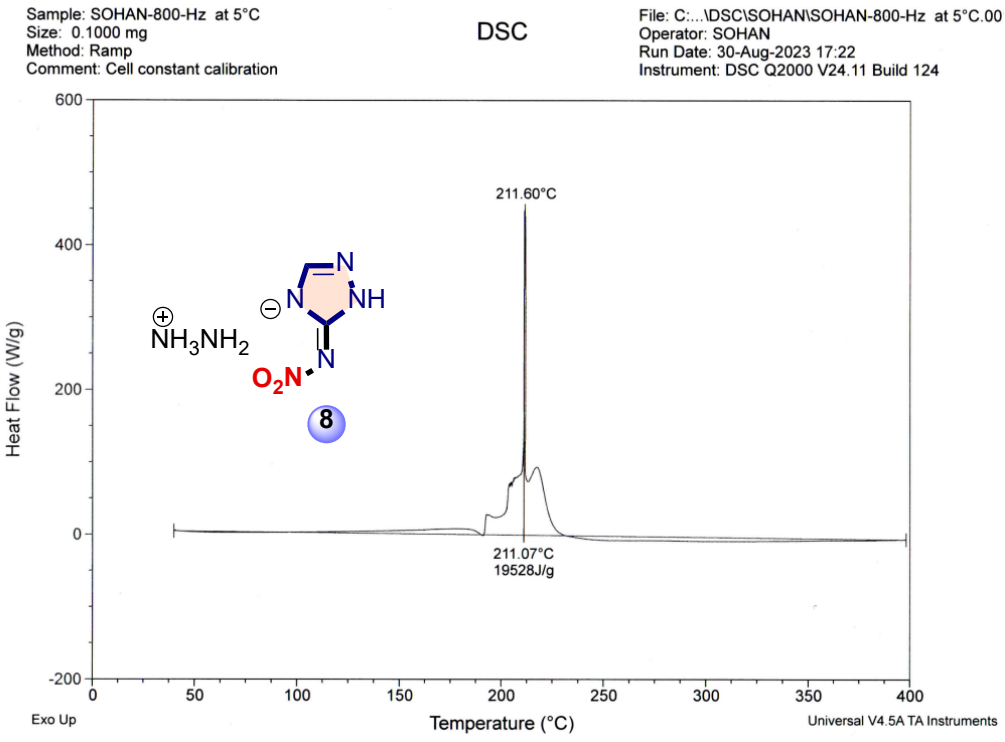


Fig. S53. DSC of compound **8** at 5 °C min^{-1}

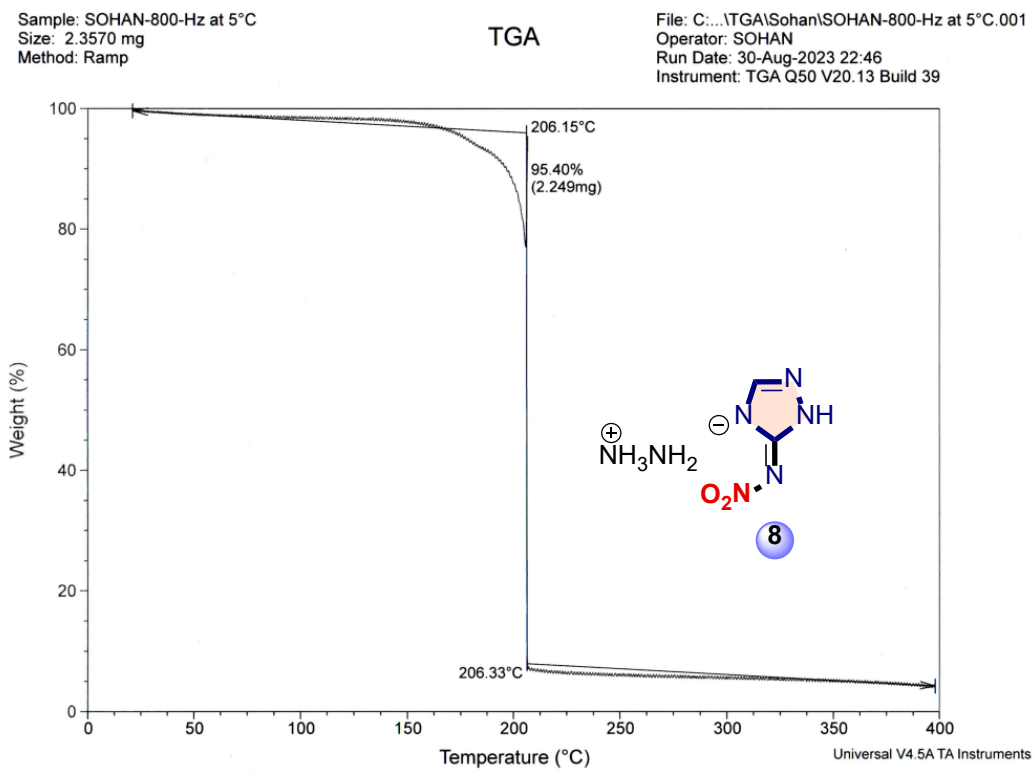


Fig. S54. TGA of compound **8** at 5 °C min^{-1}

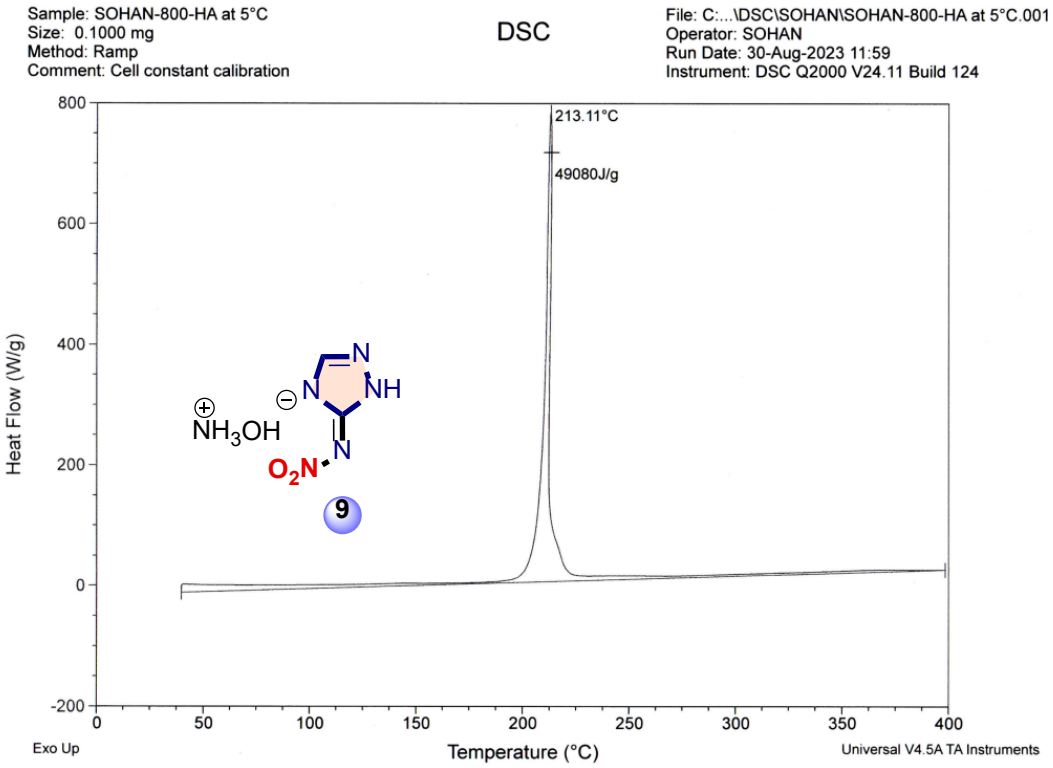


Fig. S55. DSC of compound **9** at 5 °C min^{-1}

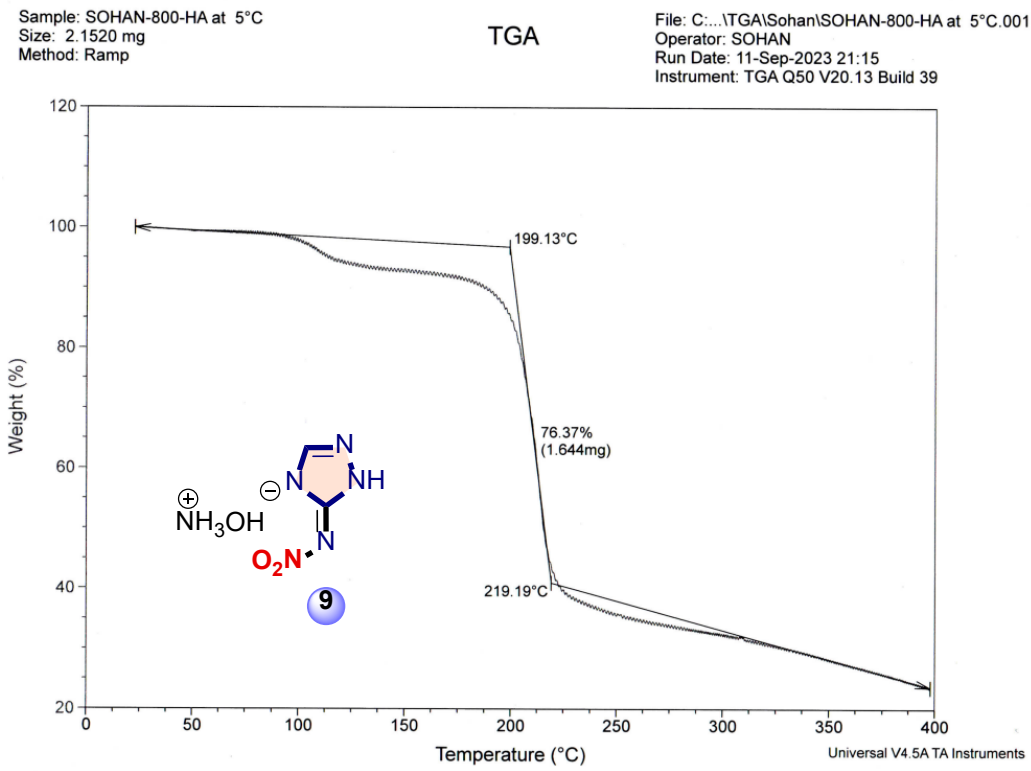


Fig. S56. TGA of compound **9** at 5 °C min^{-1}

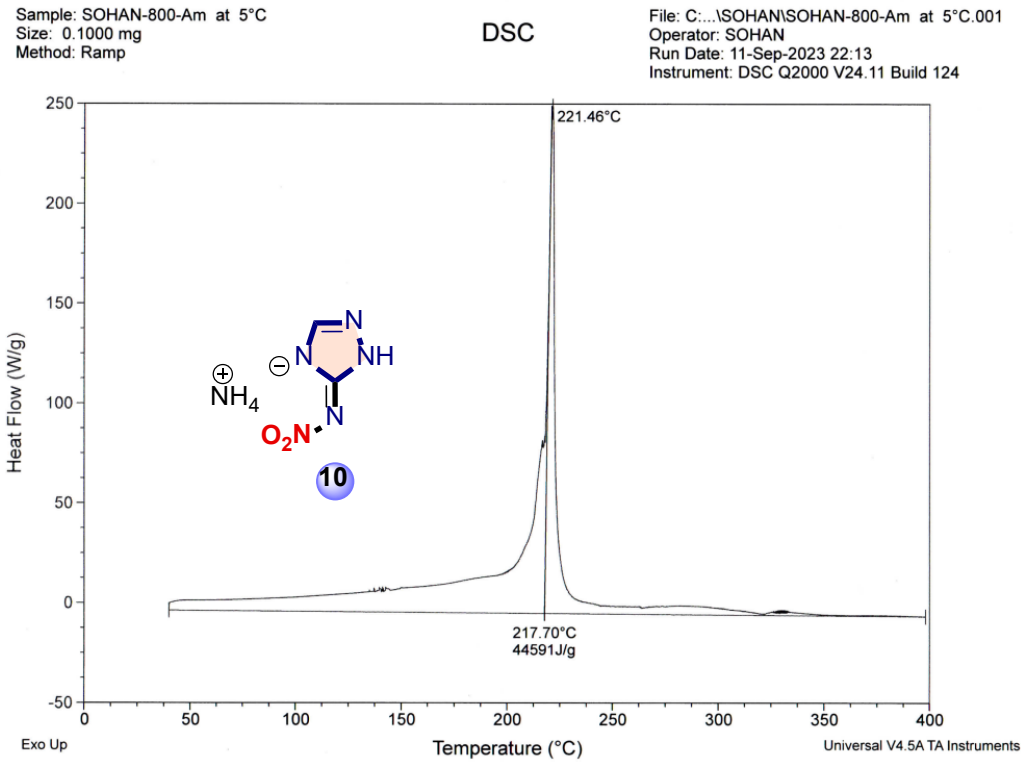


Fig. S57. DSC of compound **10** at 5 °C min^{-1}

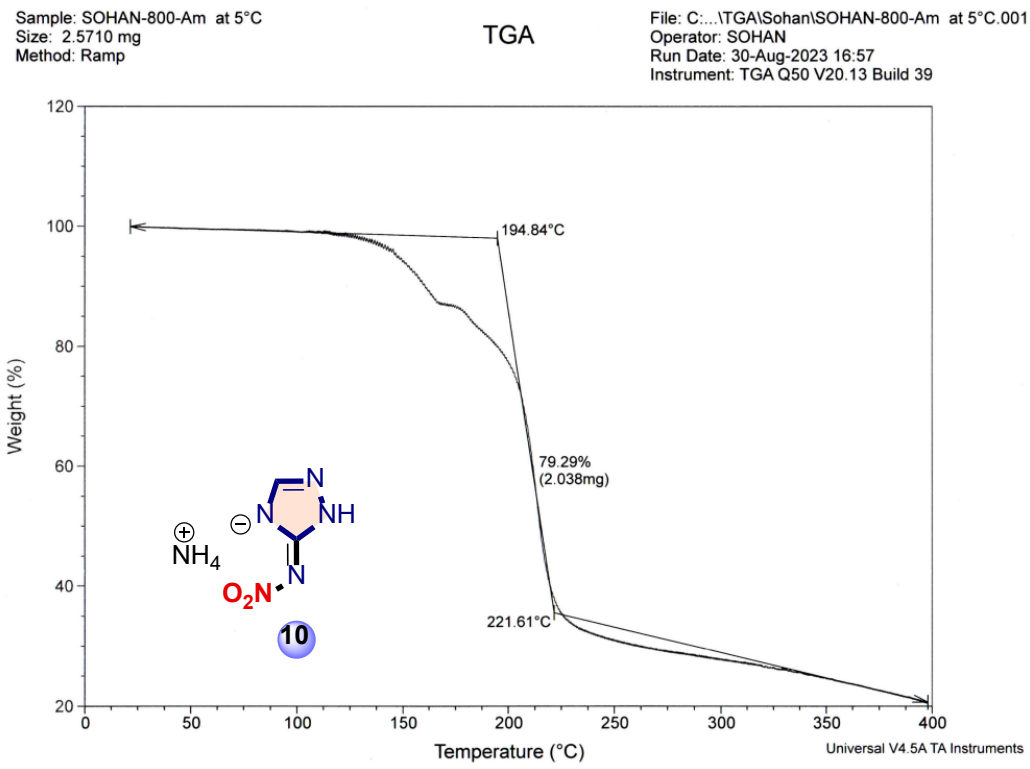


Fig. S58. TGA of compound **10** at 5 °C min^{-1}

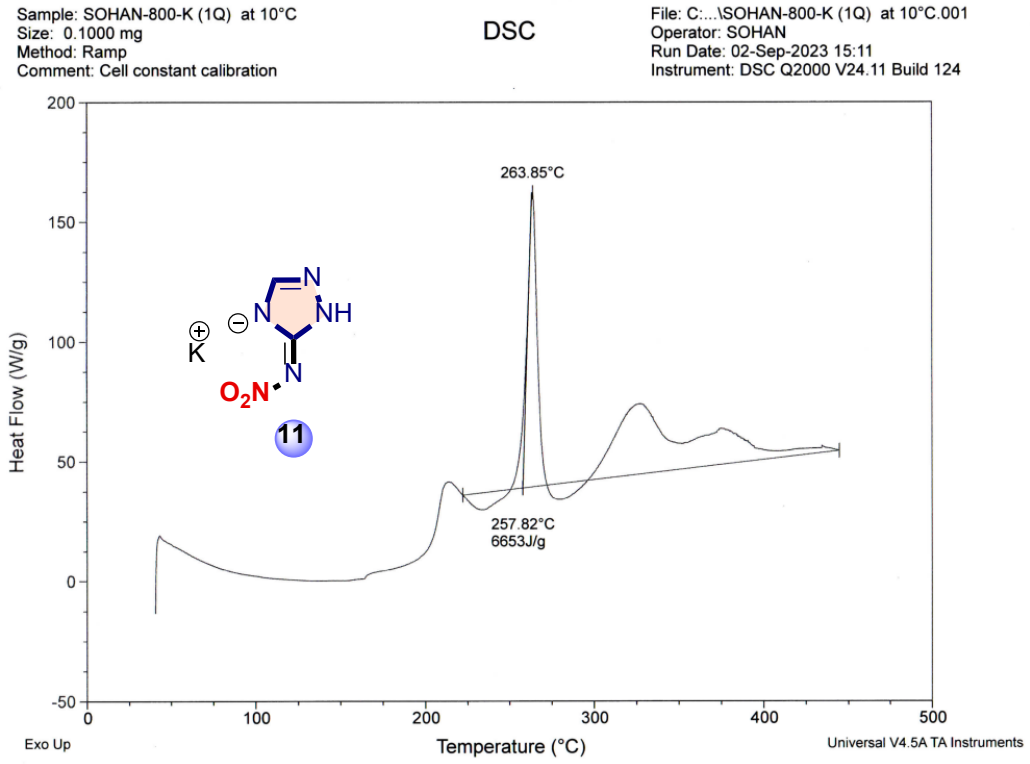


Fig. S59. DSC of compound **11** at 5 °C min^{-1}

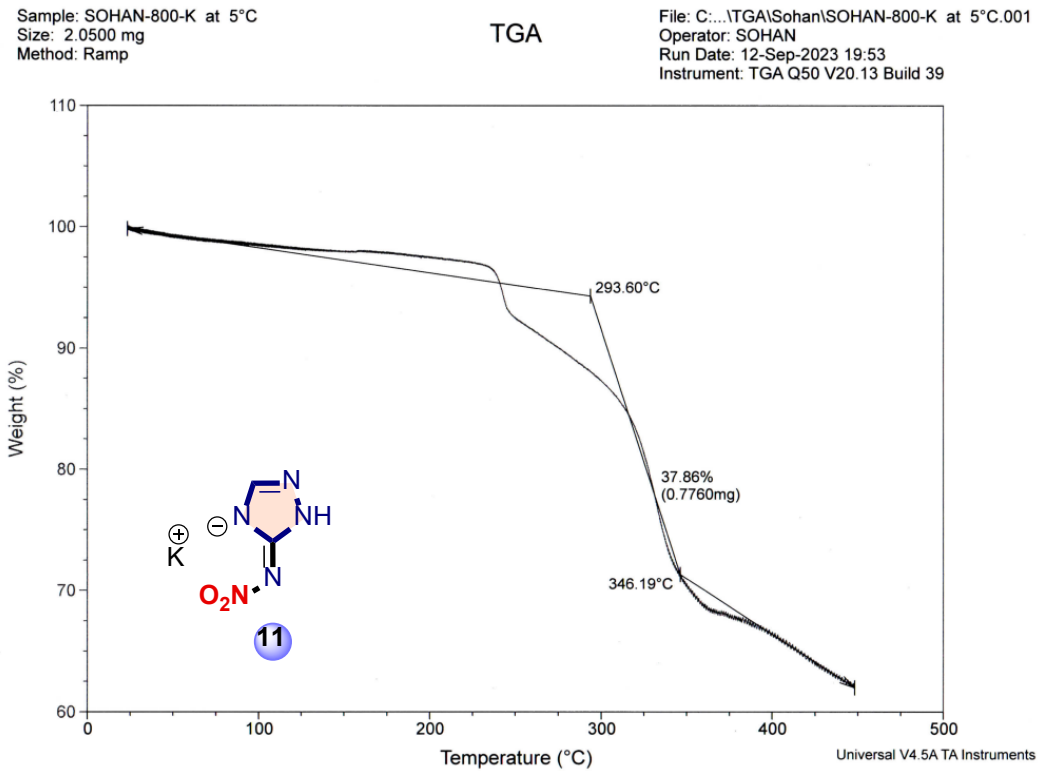


Fig. S60. TGA of compound **11** at 5 °C min^{-1}

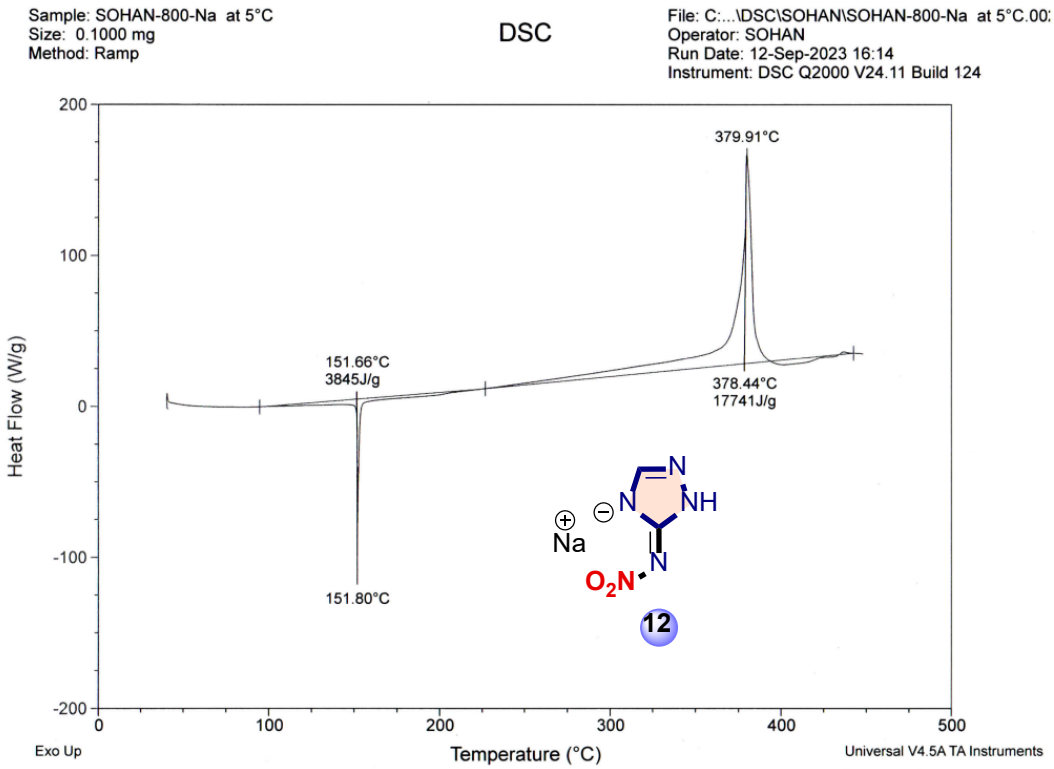


Fig. S61. DSC of compound **12** at 5 °C min^{-1}

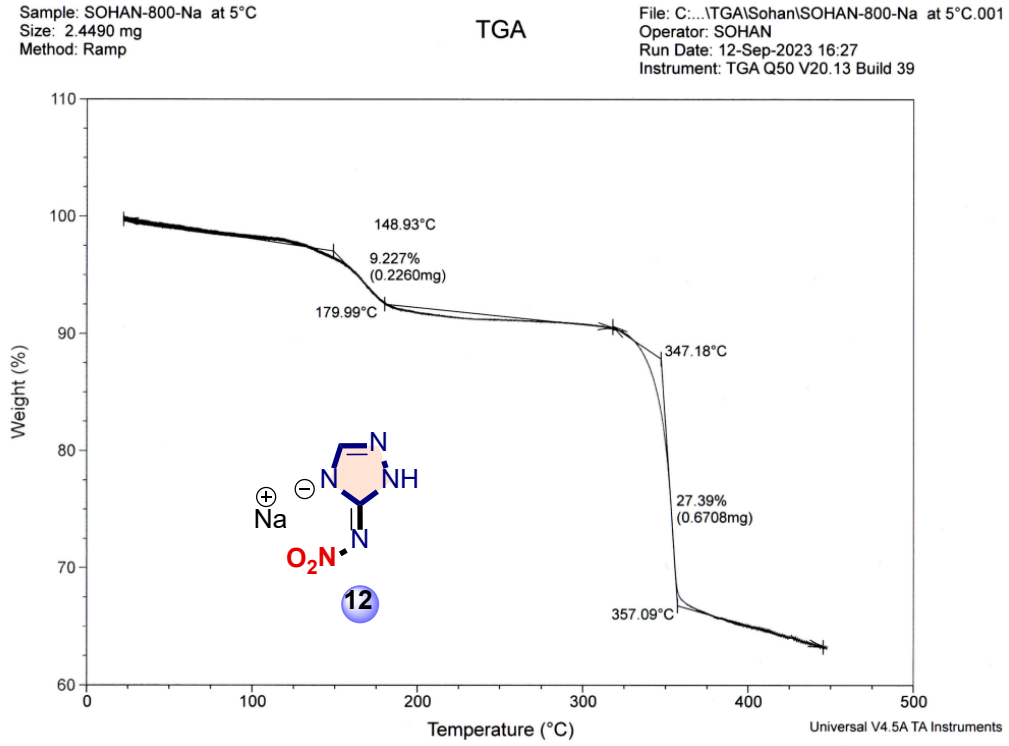


Fig. S62. TGA of compound **12** at 5 °C min^{-1}

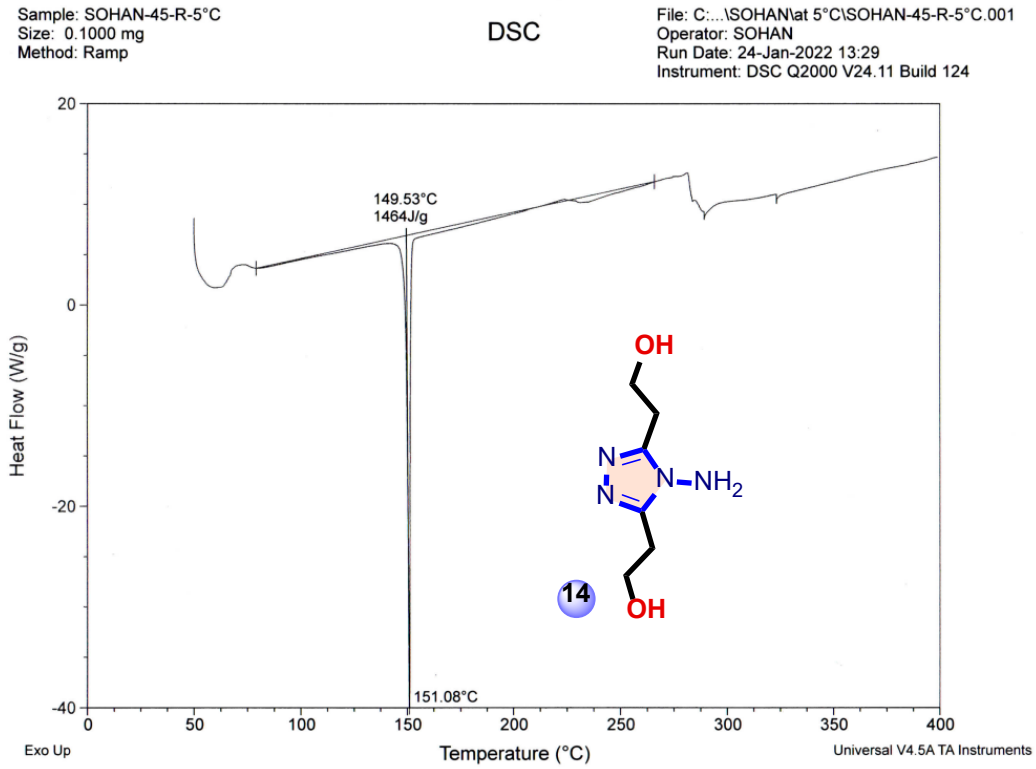


Fig. S63. DSC of compound **14** at 5 °C min^{-1}

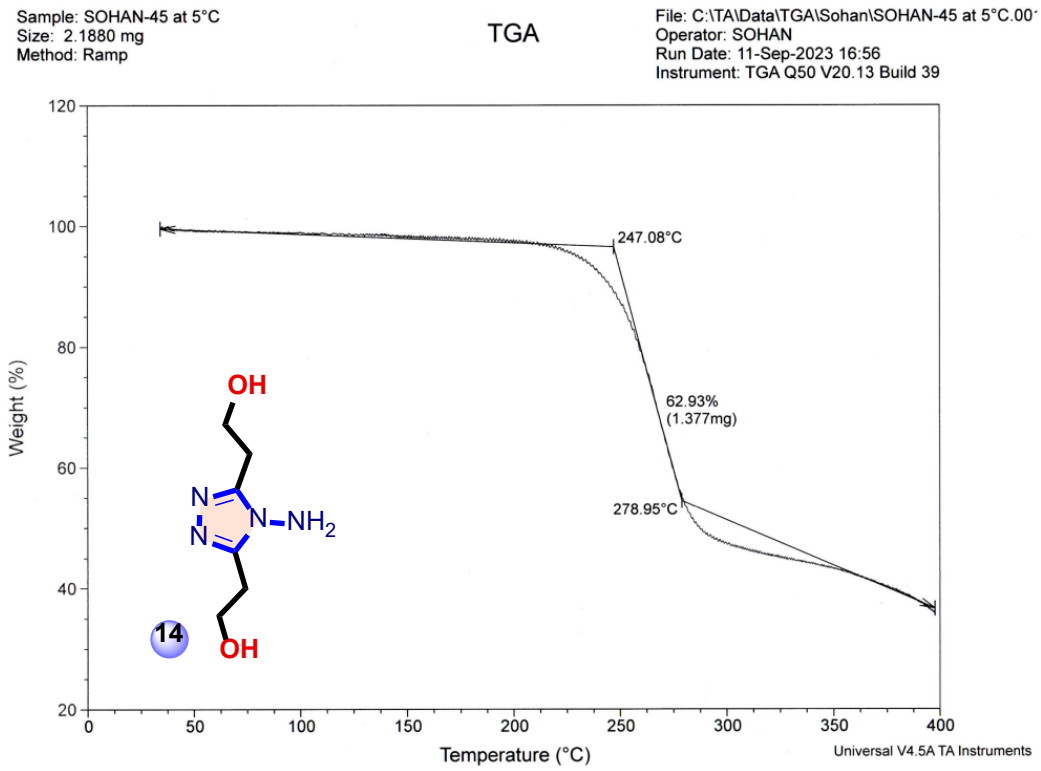


Fig. S64. TGA of compound **14** at 5 °C min^{-1}

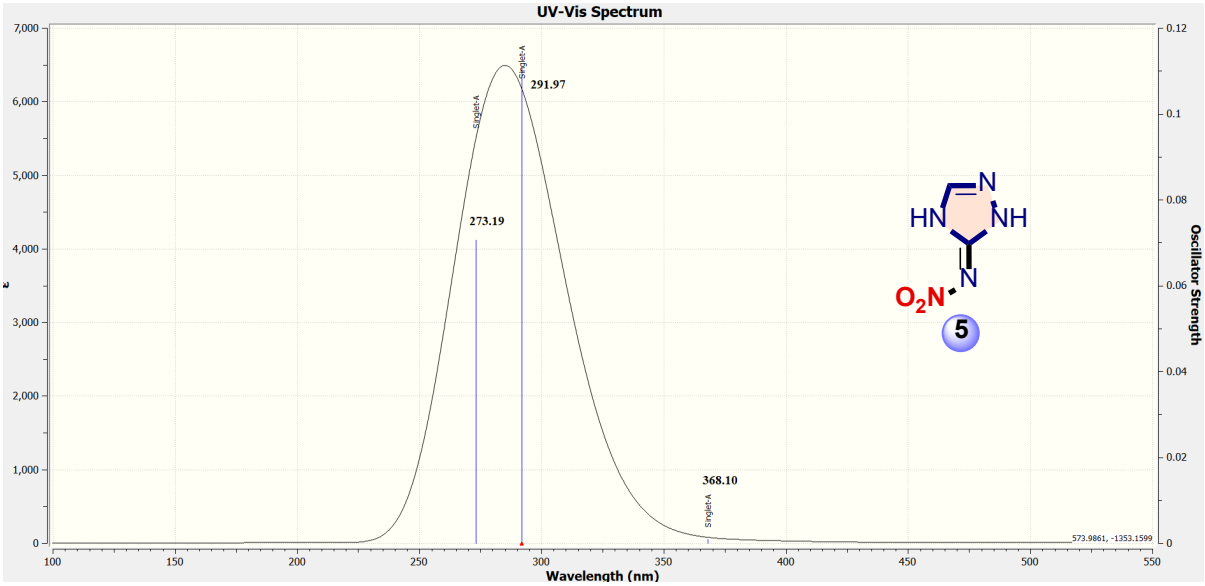


Figure S65. Predicted UV-Visible spectrum of **5** at B3LYP/6-311++G(d,p) level.

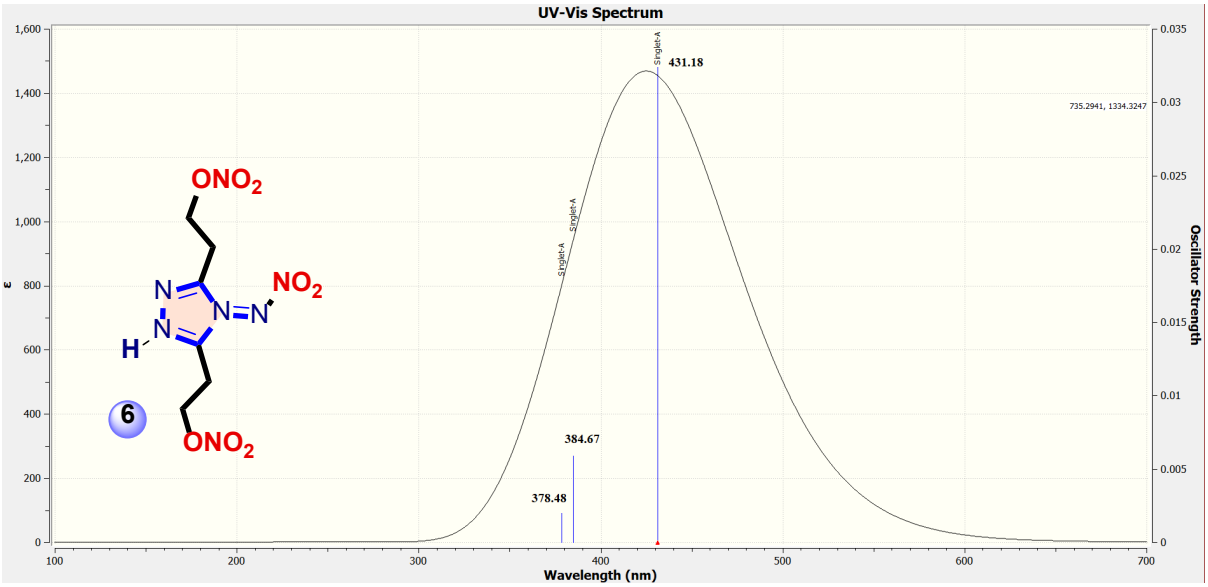


Figure S66. Predicted UV-Visible spectrum of **6** at B3LYP/6-311++G(d,p) level.

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